Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:16 PM GMT

PDB ID	:	3WN5
Title	:	Crystal structure of asymmetrically engineered Fc variant in complex with FcgRIIIa
Authors	:	Kadono, S.; Mimoto, F.; Katada, H.; Igawa, T.; Kamikawa, T.; Hattori, K.
Deposited on	:	2013-12-05
Resolution	:	2.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

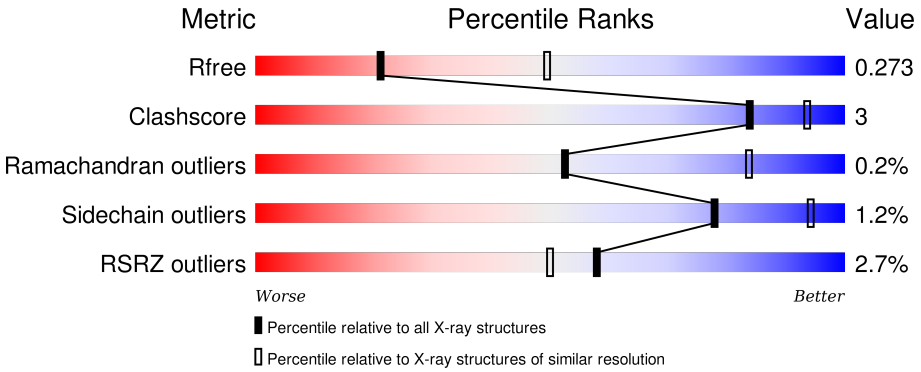
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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 <=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	230	2% 85% 7% 8%
1	D	230	% 86% 6% 8%
2	B	230	2% 78% 12% • 9%
2	E	230	5% 83% 8% 9%
3	C	197	2% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
3	F	197	2% 80% 6% 14%

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
4	GAL	A	1006	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9947 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 gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1664	1057	277	323	7			
1	D	212	Total	C	N	O	S	0	0	0
			1646	1046	274	319	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	CYS	ENGINEERED MUTATION	UNP P01857
A	270	GLU	ASP	ENGINEERED MUTATION	UNP P01857
A	326	ASP	LYS	ENGINEERED MUTATION	UNP P01857
A	330	LYS	ALA	ENGINEERED MUTATION	UNP P01857
A	334	GLU	LYS	ENGINEERED MUTATION	UNP P01857
A	356	CYS	ASP	ENGINEERED MUTATION	UNP P01857
A	366	SER	THR	ENGINEERED MUTATION	UNP P01857
A	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
A	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857
D	220	SER	CYS	ENGINEERED MUTATION	UNP P01857
D	270	GLU	ASP	ENGINEERED MUTATION	UNP P01857
D	326	ASP	LYS	ENGINEERED MUTATION	UNP P01857
D	330	LYS	ALA	ENGINEERED MUTATION	UNP P01857
D	334	GLU	LYS	ENGINEERED MUTATION	UNP P01857
D	356	CYS	ASP	ENGINEERED MUTATION	UNP P01857
D	366	SER	THR	ENGINEERED MUTATION	UNP P01857
D	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
D	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1664	1065	271	320	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	210	Total	C	N	O	S	0	0	0
			1644	1056	267	313	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	SER	CYS	ENGINEERED MUTATION	UNP P01857
B	234	TYR	LEU	ENGINEERED MUTATION	UNP P01857
B	235	TYR	LEU	ENGINEERED MUTATION	UNP P01857
B	236	TRP	GLY	ENGINEERED MUTATION	UNP P01857
B	239	MET	SER	ENGINEERED MUTATION	UNP P01857
B	268	ASP	HIS	ENGINEERED MUTATION	UNP P01857
B	298	ALA	SER	ENGINEERED MUTATION	UNP P01857
B	327	ASP	ALA	ENGINEERED MUTATION	UNP P01857
B	349	CYS	TYR	ENGINEERED MUTATION	UNP P01857
B	366	TRP	THR	ENGINEERED MUTATION	UNP P01857
E	220	SER	CYS	ENGINEERED MUTATION	UNP P01857
E	234	TYR	LEU	ENGINEERED MUTATION	UNP P01857
E	235	TYR	LEU	ENGINEERED MUTATION	UNP P01857
E	236	TRP	GLY	ENGINEERED MUTATION	UNP P01857
E	239	MET	SER	ENGINEERED MUTATION	UNP P01857
E	268	ASP	HIS	ENGINEERED MUTATION	UNP P01857
E	298	ALA	SER	ENGINEERED MUTATION	UNP P01857
E	327	ASP	ALA	ENGINEERED MUTATION	UNP P01857
E	349	CYS	TYR	ENGINEERED MUTATION	UNP P01857
E	366	TRP	THR	ENGINEERED MUTATION	UNP P01857

- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	169	Total	C	N	O	S	0	0	0
			1358	867	232	255	4			
3	F	170	Total	C	N	O	S	0	0	0
			1354	862	230	258	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLN	ASN	ENGINEERED MUTATION	UNP P08637
C	71	GLN	ASN	ENGINEERED MUTATION	UNP P08637
C	155	VAL	PHE	SEE REMARK 999	UNP P08637
C	166	GLN	ASN	ENGINEERED MUTATION	UNP P08637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	188	HIS	-	EXPRESSION TAG	UNP P08637
C	189	HIS	-	EXPRESSION TAG	UNP P08637
C	190	HIS	-	EXPRESSION TAG	UNP P08637
C	191	HIS	-	EXPRESSION TAG	UNP P08637
C	192	HIS	-	EXPRESSION TAG	UNP P08637
C	193	HIS	-	EXPRESSION TAG	UNP P08637
F	35	GLN	ASN	ENGINEERED MUTATION	UNP P08637
F	71	GLN	ASN	ENGINEERED MUTATION	UNP P08637
F	155	VAL	PHE	SEE REMARK 999	UNP P08637
F	166	GLN	ASN	ENGINEERED MUTATION	UNP P08637
F	188	HIS	-	EXPRESSION TAG	UNP P08637
F	189	HIS	-	EXPRESSION TAG	UNP P08637
F	190	HIS	-	EXPRESSION TAG	UNP P08637
F	191	HIS	-	EXPRESSION TAG	UNP P08637
F	192	HIS	-	EXPRESSION TAG	UNP P08637
F	193	HIS	-	EXPRESSION TAG	UNP P08637

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	9	Total	C	N	O	0	0
			110	62	4	44		
4	B	9	Total	C	N	O	0	0
			110	62	4	44		
4	E	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	I	0	0
			1	1		
5	E	4	Total	I	0	0
			4	4		
5	B	3	Total	I	0	0
			3	3		
5	C	2	Total	I	0	0
			2	2		
5	A	2	Total	I	0	0
			2	2		
5	F	4	Total	I	0	0
			4	4		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

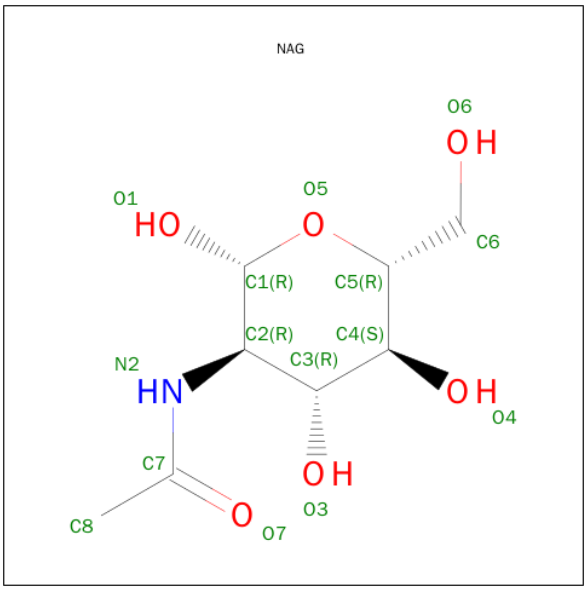
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	C	2	28	16	2	10	0	0
7	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	D	8	99	56	4	39	0	0

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

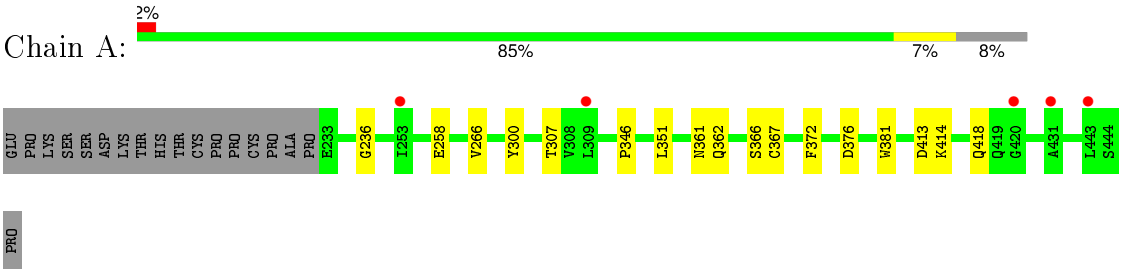
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	7	Total O 7 7	0	0
10	B	11	Total O 11 11	0	0
10	C	6	Total O 6 6	0	0
10	D	4	Total O 4 4	0	0
10	E	3	Total O 3 3	0	0
10	F	10	Total O 10 10	0	0

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.

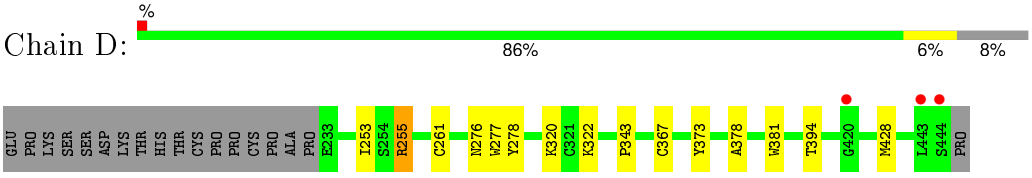
• Molecule 1: Ig gamma-1 chain C region

Chain A:



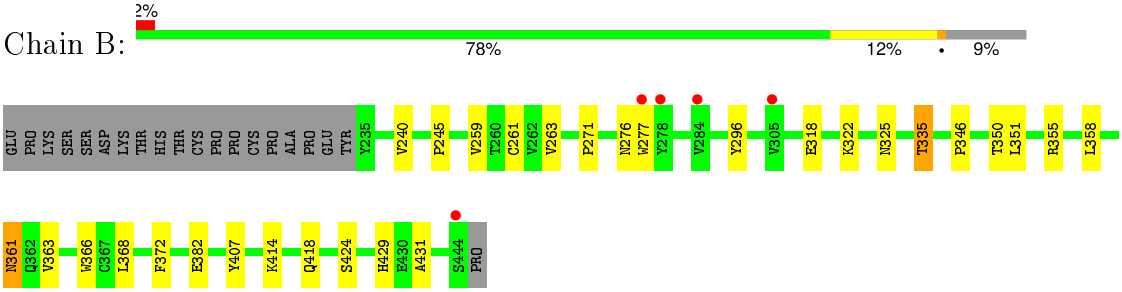
• Molecule 1: Ig gamma-1 chain C region

Chain D:



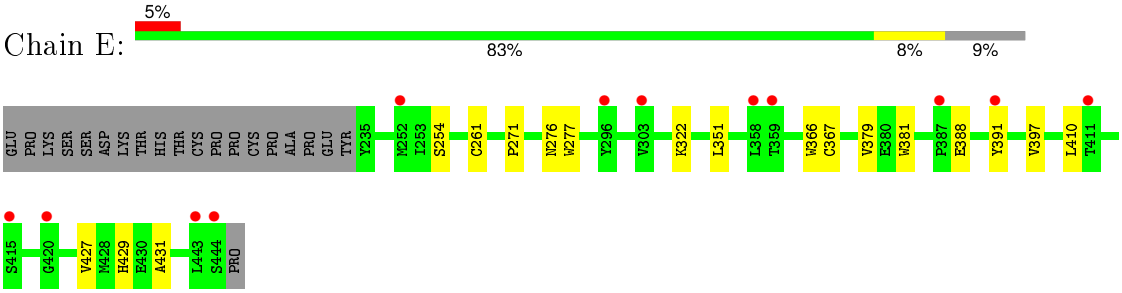
• Molecule 2: Ig gamma-1 chain C region

Chain B:



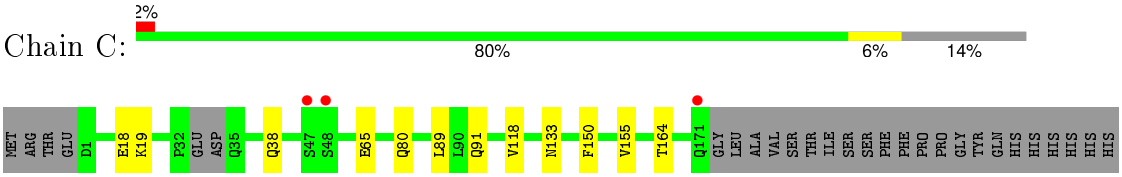
• Molecule 2: Ig gamma-1 chain C region

Chain E:



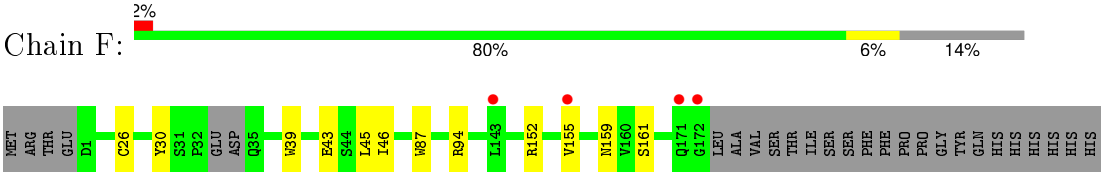
• Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C:



• Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.03Å 72.49Å 163.48Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.78 44.51 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.78) 98.1 (44.51-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.236 , 0.274 0.236 , 0.273	Depositor DCC
R_{free} test set	2186 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.0	EDS
Estimated twinning fraction	0.015 for k,h,-l 0.016 for -k,-h,-l 0.020 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 43596 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, GAL, FUL, IOD, 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	0.28	0/1709	0.46	0/2334
1	D	0.28	0/1691	0.46	0/2313
2	B	0.28	0/1713	0.46	0/2343
2	E	0.28	0/1693	0.44	0/2318
3	C	0.30	0/1395	0.49	0/1897
3	F	0.29	0/1391	0.48	0/1895
All	All	0.28	0/9592	0.46	0/13100

There are no bond length outliers.

There are no bond angle outliers.

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	1664	0	1594	8	0
1	D	1646	0	1567	11	0
2	B	1664	0	1580	16	0
2	E	1644	0	1547	11	0
3	C	1358	0	1299	7	0
3	F	1354	0	1273	4	0
4	A	110	0	94	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	110	0	94	2	0
4	E	110	0	94	0	0
5	A	2	0	0	0	0
5	B	3	0	0	1	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
6	C	61	0	52	0	0
7	C	28	0	25	0	0
7	F	28	0	25	0	0
8	D	99	0	85	0	0
9	F	14	0	13	0	0
10	A	7	0	0	0	0
10	B	11	0	0	0	0
10	C	6	0	0	0	0
10	D	4	0	0	0	0
10	E	3	0	0	0	0
10	F	10	0	0	0	0
All	All	9947	0	9342	57	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 3.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.47	0.80
1:D:255:ARG:CG	1:D:255:ARG:HH11	2.04	0.71
2:B:296:TYR:H	4:B:1007:FUL:H61	1.57	0.69
3:F:152:ARG:HB3	3:F:161:SER:HB3	1.75	0.68
2:E:351:LEU:HB2	2:E:366:TRP:HB2	1.81	0.61
2:B:276:ASN:HB2	2:B:322:LYS:HB3	1.83	0.61
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.39	0.58
4:A:1005:NAG:H4	4:A:1006:GAL:O2	2.03	0.58
3:C:65:GLU:HG2	3:C:80:GLN:HE22	1.69	0.57
1:A:351:LEU:HB2	1:A:366:SER:HB2	1.85	0.57
1:D:276:ASN:HB2	1:D:322:LYS:HB3	1.87	0.56
2:B:318:GLU:HG3	2:B:335:THR:CG2	2.36	0.56
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.88	0.55
1:D:255:ARG:CG	1:D:255:ARG:NH1	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.43	0.54
2:E:276:ASN:HB2	2:E:322:LYS:HB3	1.91	0.52
2:B:351:LEU:HB2	2:B:366:TRP:HB2	1.94	0.50
2:E:388:GLU:HG2	2:E:410:LEU:HD11	1.94	0.50
4:B:1002:NAG:H82	4:B:1007:FUL:H2	1.94	0.49
2:E:429:HIS:CD2	2:E:431:ALA:H	2.30	0.49
2:B:361:ASN:N	2:B:361:ASN:OD1	2.37	0.49
2:E:367:CYS:HB2	2:E:381:TRP:CZ2	2.47	0.48
2:B:429:HIS:CD2	2:B:431:ALA:H	2.31	0.48
2:B:355:ARG:HA	2:B:358:LEU:HD12	1.96	0.48
2:B:245:PRO:HD3	2:B:259:VAL:HG22	1.96	0.48
2:B:346:PRO:HB3	2:B:372:PHE:HB3	1.95	0.48
1:A:258:GLU:HG2	1:A:307:THR:HG22	1.96	0.48
2:E:379:VAL:HG22	2:E:427:VAL:HG22	1.95	0.48
2:B:414:LYS:HE3	2:B:418:GLN:HE21	1.79	0.47
1:D:278:TYR:HB2	1:D:320:LYS:HB3	1.95	0.47
1:A:414:LYS:O	1:A:418:GLN:HG2	2.14	0.47
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.96	0.47
2:B:350:THR:OG1	5:B:1010:IOD:I	3.01	0.47
2:E:254:SER:OG	5:E:1011:IOD:I	2.93	0.47
3:F:87:TRP:CZ3	3:F:155:VAL:HG11	2.49	0.46
3:C:118:VAL:HG21	3:C:133:ASN:HA	1.98	0.46
1:D:253:ILE:HD12	1:D:253:ILE:H	1.81	0.45
3:C:65:GLU:HG2	3:C:80:GLN:NE2	2.32	0.45
1:A:236:GLY:HA2	3:C:155:VAL:HG12	1.99	0.45
3:F:26:CYS:HB2	3:F:39:TRP:CZ2	2.52	0.44
2:E:429:HIS:HD2	2:E:431:ALA:H	1.65	0.44
2:E:261:CYS:HB2	2:E:277:TRP:CH2	2.52	0.43
2:B:240:VAL:HG22	2:B:263:VAL:HG22	2.01	0.43
2:B:368:LEU:HD13	2:B:407:TYR:CZ	2.52	0.43
3:C:89:LEU:HD23	3:C:91:GLN:HE21	1.84	0.43
3:C:150:PHE:HB3	3:C:164:THR:HG22	2.01	0.43
3:C:18:GLU:O	3:C:19:LYS:HB2	2.17	0.43
1:D:261:CYS:HB2	1:D:277:TRP:CZ2	2.54	0.42
2:E:391:TYR:HB3	2:E:410:LEU:HD12	2.00	0.42
1:D:394:THR:HG22	2:E:397:VAL:HG21	2.02	0.41
3:F:30:TYR:O	5:F:206:IOD:I	3.08	0.41
1:A:362:GLN:HG2	1:A:413:ASP:HA	2.02	0.41
1:D:343:PRO:HA	1:D:373:TYR:O	2.21	0.41
2:B:261:CYS:HB2	2:B:277:TRP:CH2	2.55	0.41
2:B:382:GLU:HG2	2:B:424:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLU:HG3	2:B:335:THR:HG22	2.02	0.41
1:D:378:ALA:HB3	1:D:428:MET:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
1	D	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
2	B	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	34	68
2	E	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	34	68
3	C	165/197 (84%)	162 (98%)	3 (2%)	0	100	100
3	F	166/197 (84%)	162 (98%)	4 (2%)	0	100	100
All	All	1167/1314 (89%)	1130 (97%)	35 (3%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	PRO
2	E	271	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/214 (89%)	188 (99%)	2 (1%)	80 95
1	D	187/214 (87%)	186 (100%)	1 (0%)	92 98
2	B	188/215 (87%)	184 (98%)	4 (2%)	61 88
2	E	181/215 (84%)	181 (100%)	0	100 100
3	C	150/178 (84%)	149 (99%)	1 (1%)	88 97
3	F	148/178 (83%)	143 (97%)	5 (3%)	44 77
All	All	1044/1214 (86%)	1031 (99%)	13 (1%)	78 94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	376	ASP
2	B	325	ASN
2	B	335	THR
2	B	361	ASN
2	B	363	VAL
3	C	38	GLN
1	D	255	ARG
3	F	43	GLU
3	F	45	LEU
3	F	46	ILE
3	F	94	ARG
3	F	159	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	362	GLN
2	B	325	ASN
2	B	418	GLN
2	B	429	HIS
3	C	69	GLN
3	C	71	GLN
3	C	80	GLN
3	C	171	GLN
1	D	315	ASN
1	D	347	GLN
2	E	315	ASN

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Mol	Chain	Res	Type
2	E	347	GLN
2	E	418	GLN
2	E	429	HIS
3	F	12	GLN
3	F	69	GLN
3	F	108	HIS

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

44 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	$\#\|Z\| > 2$
4	NAG	A	1001	1,4	14,14,15	0.45	0	15,19,21	1.22	2 (13%)
4	NAG	A	1002	4	14,14,15	0.55	0	15,19,21	0.79	0
4	BMA	A	1003	4	11,11,12	0.45	0	14,15,17	0.81	0
4	MAN	A	1004	4	11,11,12	0.53	0	14,15,17	0.99	1 (7%)
4	NAG	A	1005	4	14,14,15	0.51	0	15,19,21	0.71	0
4	GAL	A	1006	4	11,11,12	0.57	0	14,15,17	1.27	1 (7%)
4	FUL	A	1007	4	10,10,11	0.64	0	14,14,16	1.69	4 (28%)
4	MAN	A	1008	4	11,11,12	0.55	0	14,15,17	0.90	0
4	NAG	A	1009	4	14,14,15	0.45	0	15,19,21	0.76	0
4	NAG	B	1001	2,4	14,14,15	0.56	0	15,19,21	0.86	1 (6%)
4	NAG	B	1002	4	14,14,15	0.48	0	15,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	B	1003	4	11,11,12	0.57	0	14,15,17	1.28	2 (14%)
4	MAN	B	1004	4	11,11,12	0.53	0	14,15,17	0.88	1 (7%)
4	NAG	B	1005	4	14,14,15	0.56	0	15,19,21	1.18	1 (6%)
4	GAL	B	1006	4	11,11,12	0.57	0	14,15,17	0.76	0
4	FUL	B	1007	4	10,10,11	0.44	0	14,14,16	1.10	2 (14%)
4	MAN	B	1008	4	11,11,12	0.48	0	14,15,17	1.72	3 (21%)
4	NAG	B	1009	4	14,14,15	0.57	0	15,19,21	1.06	1 (6%)
6	NAG	C	201	3,6	14,14,15	0.46	0	15,19,21	2.03	2 (13%)
6	NAG	C	202	6	14,14,15	0.47	0	15,19,21	0.78	0
6	BMA	C	203	6	11,11,12	0.44	0	14,15,17	0.79	0
6	MAN	C	204	6	11,11,12	0.58	0	14,15,17	1.01	1 (7%)
6	MAN	C	205	6	11,11,12	0.57	0	14,15,17	1.25	2 (14%)
7	NAG	C	206	3,7	14,14,15	0.46	0	15,19,21	0.94	1 (6%)
7	NAG	C	207	7	14,14,15	0.43	0	15,19,21	0.95	1 (6%)
8	NAG	D	1001	1,8	14,14,15	0.50	0	15,19,21	0.96	0
8	NAG	D	1002	8	14,14,15	0.51	0	15,19,21	0.69	0
8	BMA	D	1003	8	11,11,12	0.43	0	14,15,17	1.24	2 (14%)
8	MAN	D	1004	8	11,11,12	0.58	0	14,15,17	0.88	1 (7%)
8	NAG	D	1005	8	14,14,15	0.48	0	15,19,21	0.71	0
8	FUL	D	1006	8	10,10,11	0.46	0	14,14,16	0.75	0
8	MAN	D	1007	8	11,11,12	0.51	0	14,15,17	0.89	1 (7%)
8	NAG	D	1008	8	14,14,15	0.47	0	15,19,21	0.74	0
4	NAG	E	1001	2,4	14,14,15	0.42	0	15,19,21	1.41	1 (6%)
4	NAG	E	1002	4	14,14,15	0.45	0	15,19,21	0.79	0
4	BMA	E	1003	4	11,11,12	0.46	0	14,15,17	0.85	1 (7%)
4	MAN	E	1004	4	11,11,12	0.55	0	14,15,17	0.98	1 (7%)
4	NAG	E	1005	4	14,14,15	0.51	0	15,19,21	0.75	0
4	GAL	E	1006	4	11,11,12	0.62	0	14,15,17	0.63	0
4	FUL	E	1007	4	10,10,11	0.50	0	14,14,16	0.86	1 (7%)
4	MAN	E	1008	4	11,11,12	0.46	0	14,15,17	1.24	1 (7%)
4	NAG	E	1009	4	14,14,15	0.56	0	15,19,21	0.95	1 (6%)
7	NAG	F	202	3,7	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
7	NAG	F	203	7	14,14,15	0.46	0	15,19,21	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1005	4	-	0/6/23/26	0/1/1/1
4	GAL	A	1006	4	-	0/2/19/22	0/1/1/1
4	FUL	A	1007	4	-	0/0/17/20	0/1/1/1
4	MAN	A	1008	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1009	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1004	4	-	0/2/19/22	0/1/1/1
4	NAG	B	1005	4	-	0/6/23/26	0/1/1/1
4	GAL	B	1006	4	-	0/2/19/22	0/1/1/1
4	FUL	B	1007	4	-	0/0/17/20	0/1/1/1
4	MAN	B	1008	4	-	0/2/19/22	0/1/1/1
4	NAG	B	1009	4	-	0/6/23/26	0/1/1/1
6	NAG	C	201	3,6	-	0/6/23/26	0/1/1/1
6	NAG	C	202	6	-	0/6/23/26	0/1/1/1
6	BMA	C	203	6	-	0/2/19/22	0/1/1/1
6	MAN	C	204	6	-	0/2/19/22	0/1/1/1
6	MAN	C	205	6	-	0/2/19/22	0/1/1/1
7	NAG	C	206	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	207	7	-	0/6/23/26	0/1/1/1
8	NAG	D	1001	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1002	8	-	0/6/23/26	0/1/1/1
8	BMA	D	1003	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1004	8	-	0/2/19/22	0/1/1/1
8	NAG	D	1005	8	-	0/6/23/26	0/1/1/1
8	FUL	D	1006	8	-	0/0/17/20	0/1/1/1
8	MAN	D	1007	8	-	0/2/19/22	0/1/1/1
8	NAG	D	1008	8	-	0/6/23/26	0/1/1/1
4	NAG	E	1001	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	E	1004	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1005	4	-	0/6/23/26	0/1/1/1
4	GAL	E	1006	4	-	0/2/19/22	0/1/1/1
4	FUL	E	1007	4	-	0/0/17/20	0/1/1/1
4	MAN	E	1008	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1009	4	-	0/6/23/26	0/1/1/1
7	NAG	F	202	3,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	F	203	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1008	MAN	O2-C2-C3	-2.86	104.36	110.12
4	E	1003	BMA	C1-C2-C3	2.03	111.94	109.54
6	C	204	MAN	C1-C2-C3	2.08	112.00	109.54
4	A	1001	NAG	O5-C5-C6	2.27	112.26	107.35
6	C	205	MAN	C3-C4-C5	2.28	114.16	110.20
4	A	1007	FUL	O5-C5-C6	2.29	109.91	106.13
7	F	202	NAG	C1-O5-C5	2.30	115.17	112.25
4	B	1004	MAN	C1-O5-C5	2.33	115.21	112.25
4	B	1007	FUL	C1-C2-C3	2.35	112.32	109.54
8	D	1004	MAN	C1-O5-C5	2.35	115.24	112.25
4	B	1001	NAG	C1-O5-C5	2.40	115.29	112.25
4	E	1007	FUL	O5-C5-C6	2.45	110.18	106.13
4	B	1009	NAG	C4-C3-C2	2.46	115.06	111.23
4	A	1007	FUL	O5-C5-C4	2.48	113.82	109.53
4	E	1009	NAG	C3-C4-C5	2.51	114.57	110.20
8	D	1007	MAN	C1-O5-C5	2.56	115.50	112.25
7	C	206	NAG	C1-O5-C5	2.69	115.66	112.25
7	F	203	NAG	C1-O5-C5	2.69	115.67	112.25
7	C	207	NAG	C1-O5-C5	2.72	115.71	112.25
4	B	1007	FUL	O5-C5-C6	2.76	110.70	106.13
8	D	1003	BMA	C1-C2-C3	2.77	112.82	109.54
4	B	1003	BMA	C1-O5-C5	2.80	115.80	112.25
4	E	1004	MAN	C1-O5-C5	2.82	115.83	112.25
4	A	1001	NAG	C1-O5-C5	2.87	115.89	112.25
4	B	1008	MAN	O2-C2-C1	2.92	115.05	109.21
4	A	1004	MAN	C1-O5-C5	2.98	116.04	112.25
4	B	1003	BMA	C1-C2-C3	3.00	113.08	109.54
4	A	1007	FUL	C3-C4-C5	3.24	115.19	109.72
6	C	205	MAN	C1-O5-C5	3.29	116.43	112.25
4	B	1005	NAG	C4-C3-C2	3.33	116.40	111.23
4	A	1007	FUL	C1-O5-C5	3.42	117.66	112.38
4	E	1008	MAN	C1-O5-C5	3.42	116.59	112.25
8	D	1003	BMA	C1-O5-C5	3.45	116.62	112.25
4	B	1008	MAN	C1-O5-C5	3.46	116.64	112.25
6	C	201	NAG	C2-N2-C7	3.68	127.77	123.04
4	A	1006	GAL	C1-O5-C5	3.69	116.94	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1001	NAG	C1-O5-C5	4.32	117.73	112.25
6	C	201	NAG	C1-O5-C5	6.02	119.89	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	NAG	1	0
4	A	1006	GAL	1	0
4	B	1002	NAG	1	0
4	B	1007	FUL	2	0

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
9	NAG	F	201	3	14,14,15	0.48	0	15,19,21	0.80	1 (6%)

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
9	NAG	F	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	201	NAG	C1-O5-C5	2.08	114.89	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	212/230 (92%)	0.39	5 (2%)	62	55	38, 52, 68, 79	0
1	D	212/230 (92%)	0.29	3 (1%)	78	72	37, 57, 84, 98	0
2	B	210/230 (91%)	0.40	5 (2%)	62	55	31, 48, 77, 94	0
2	E	210/230 (91%)	0.63	12 (5%)	27	20	44, 70, 111, 121	0
3	C	169/197 (85%)	0.25	3 (1%)	71	65	30, 44, 73, 98	0
3	F	170/197 (86%)	0.33	4 (2%)	62	55	30, 45, 68, 94	0
All	All	1183/1314 (90%)	0.39	32 (2%)	58	50	30, 53, 85, 121	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	47	SER	5.8
1	D	420	GLY	4.0
1	D	443	LEU	3.9
2	E	443	LEU	3.8
3	C	48	SER	3.5
3	F	171	GLN	3.2
2	E	296	TYR	3.1
2	E	444	SER	3.1
3	F	143	LEU	3.0
2	E	415	SER	2.7
2	B	444	SER	2.7
2	E	387	PRO	2.6
3	C	171	GLN	2.6
1	A	253	ILE	2.6
2	E	411	THR	2.5
2	B	278	TYR	2.4
3	F	155	VAL	2.4
3	F	172	GLY	2.4
2	E	252	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	LEU	2.3
2	B	277	TRP	2.3
2	E	420	GLY	2.3
1	A	309	LEU	2.3
1	A	420	GLY	2.2
1	A	431	ALA	2.2
2	E	358	LEU	2.2
2	E	359	THR	2.2
2	E	391	TYR	2.2
2	E	303	VAL	2.2
2	B	305	VAL	2.2
2	B	284	VAL	2.1
1	D	444	SER	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, 95^{th} 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	GAL	A	1006	11/12	0.70	0.39	3.13	77,83,85,86	0
6	NAG	C	201	14/15	0.94	0.20	1.54	47,49,53,54	0
8	NAG	D	1005	14/15	0.91	0.20	0.66	54,56,58,58	0
4	GAL	B	1006	11/12	0.91	0.21	0.33	73,74,76,78	0
4	GAL	E	1006	11/12	0.89	0.21	0.05	64,66,67,67	0
7	NAG	C	206	14/15	0.96	0.20	-0.08	57,60,63,65	0
4	NAG	A	1005	14/15	0.94	0.21	-0.33	55,58,62,68	0
8	NAG	D	1001	14/15	0.93	0.18	-0.41	49,51,54,59	0
4	NAG	E	1001	14/15	0.89	0.18	-0.43	61,64,68,72	0
4	FUL	E	1007	10/11	0.80	0.24	-0.52	75,78,79,79	0
4	NAG	B	1001	14/15	0.96	0.17	-0.87	45,50,56,61	0
4	NAG	E	1005	14/15	0.91	0.15	-1.20	56,59,61,62	0
7	NAG	F	202	14/15	0.94	0.17	-1.37	46,49,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	1005	14/15	0.92	0.18	-1.43	67,68,70,72	0
4	NAG	E	1002	14/15	0.97	0.14	-1.55	55,60,61,63	0
4	NAG	B	1002	14/15	0.93	0.17	-1.88	50,54,56,57	0
4	NAG	A	1001	14/15	0.96	0.12	-2.25	43,44,45,46	0
4	BMA	B	1003	11/12	0.93	0.17	-	57,59,61,67	0
6	MAN	C	205	11/12	0.71	0.23	-	84,86,90,93	0
4	MAN	E	1004	11/12	0.94	0.12	-	55,58,59,60	0
8	NAG	D	1002	14/15	0.96	0.19	-	47,50,53,53	0
4	FUL	B	1007	10/11	0.83	0.23	-	63,65,66,67	0
4	MAN	E	1008	11/12	0.91	0.16	-	76,80,82,89	0
8	FUL	D	1006	10/11	0.88	0.19	-	59,60,61,62	0
7	NAG	F	203	14/15	0.84	0.30	-	65,69,71,71	0
8	MAN	D	1007	11/12	0.92	0.14	-	62,64,65,68	0
4	MAN	B	1008	11/12	0.88	0.16	-	68,72,75,83	0
4	NAG	A	1009	14/15	0.91	0.20	-	52,53,56,59	0
8	BMA	D	1003	11/12	0.97	0.14	-	49,52,54,58	0
4	BMA	E	1003	11/12	0.94	0.15	-	60,63,65,71	0
4	MAN	A	1004	11/12	0.94	0.18	-	53,54,55,56	0
4	MAN	A	1008	11/12	0.93	0.17	-	51,53,55,55	0
8	MAN	D	1004	11/12	0.97	0.14	-	47,48,49,52	0
4	NAG	B	1009	14/15	0.75	0.25	-	88,91,93,93	0
4	FUL	A	1007	10/11	0.87	0.24	-	46,47,48,51	0
8	NAG	D	1008	14/15	0.83	0.23	-	71,74,75,76	0
6	NAG	C	202	14/15	0.96	0.14	-	51,57,61,67	0
4	MAN	B	1004	11/12	0.95	0.16	-	62,63,64,65	0
4	NAG	E	1009	14/15	0.66	0.34	-	96,100,107,108	0
4	NAG	A	1002	14/15	0.96	0.18	-	42,43,44,44	0
4	BMA	A	1003	11/12	0.97	0.18	-	44,46,50,51	0
6	MAN	C	204	11/12	0.86	0.26	-	82,84,86,87	0
7	NAG	C	207	14/15	0.86	0.19	-	65,68,71,72	0
6	BMA	C	203	11/12	0.91	0.13	-	71,74,78,80	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, 95^{th} 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
5	IOD	C	208	1/1	1.00	0.16	-1.31	36,36,36,36	0
5	IOD	F	204	1/1	1.00	0.17	-1.36	43,43,43,43	0
5	IOD	D	1009	1/1	0.91	0.12	-2.05	86,86,86,86	1
5	IOD	C	209	1/1	0.98	0.09	-2.64	91,91,91,91	0
5	IOD	E	1010	1/1	0.99	0.08	-3.27	102,102,102,102	0
5	IOD	B	1010	1/1	0.99	0.13	-3.89	49,49,49,49	0
5	IOD	E	1011	1/1	0.97	0.09	-5.07	85,85,85,85	0
5	IOD	F	205	1/1	0.99	0.09	-6.01	68,68,68,68	0
5	IOD	E	1013	1/1	0.96	0.07	-6.38	99,99,99,99	0
5	IOD	B	1012	1/1	0.93	0.11	-	80,80,80,80	1
5	IOD	E	1012	1/1	0.98	0.06	-	93,93,93,93	0
5	IOD	F	207	1/1	0.95	0.10	-	81,81,81,81	1
5	IOD	A	1011	1/1	0.91	0.10	-	75,75,75,75	1
5	IOD	B	1011	1/1	0.99	0.07	-	83,83,83,83	0
9	NAG	F	201	14/15	0.84	0.27	-	64,74,77,78	0
5	IOD	A	1010	1/1	0.89	0.14	-	71,71,71,71	1
5	IOD	F	206	1/1	0.97	0.09	-	58,58,58,58	1

6.5 Other polymers (i)

There are no such residues in this entry.