Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2016 – 10:44 PM EDT

PDB ID	:	5JK9
Title	:	Crystal structure of human IZUMO1
Authors	:	Ohto, U.; Ishida, H.; Shimizu, T.
Deposited on	:	2016-04-26
Resolution	:	2.10 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 (i) symbol.

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

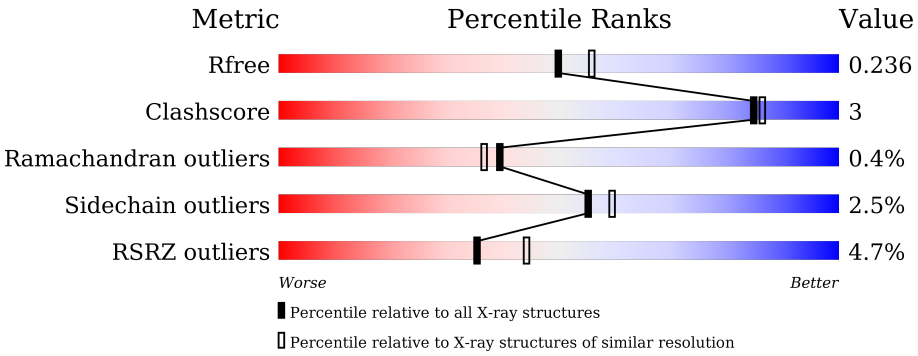
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	246	93%
1	B	246	88% 5% 6%
1	C	246	88% 9%
1	D	246	8% 74% 11% 14%
1	E	246	6% 84% 9% 6%
1	F	246	10% 92%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11717 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 Izumo sperm-egg fusion protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1925	1221	323	363	18			
1	B	231	Total	C	N	O	S	0	0	0
			1839	1167	309	345	18			
1	C	237	Total	C	N	O	S	0	1	0
			1896	1200	321	357	18			
1	D	212	Total	C	N	O	S	0	0	0
			1703	1078	291	319	15			
1	E	231	Total	C	N	O	S	0	0	0
			1838	1167	308	345	18			
1	F	238	Total	C	N	O	S	0	0	0
			1895	1200	317	360	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ARG	-	expression tag	UNP Q8IYV9
A	19	SER	-	expression tag	UNP Q8IYV9
A	20	PRO	-	expression tag	UNP Q8IYV9
A	21	TRP	-	expression tag	UNP Q8IYV9
A	256	GLU	-	expression tag	UNP Q8IYV9
A	257	PHE	-	expression tag	UNP Q8IYV9
A	258	LEU	-	expression tag	UNP Q8IYV9
A	259	GLU	-	expression tag	UNP Q8IYV9
A	260	VAL	-	expression tag	UNP Q8IYV9
A	261	LEU	-	expression tag	UNP Q8IYV9
A	262	PHE	-	expression tag	UNP Q8IYV9
A	263	GLN	-	expression tag	UNP Q8IYV9
B	18	ARG	-	expression tag	UNP Q8IYV9
B	19	SER	-	expression tag	UNP Q8IYV9
B	20	PRO	-	expression tag	UNP Q8IYV9
B	21	TRP	-	expression tag	UNP Q8IYV9
B	256	GLU	-	expression tag	UNP Q8IYV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	257	PHE	-	expression tag	UNP Q8IYV9
B	258	LEU	-	expression tag	UNP Q8IYV9
B	259	GLU	-	expression tag	UNP Q8IYV9
B	260	VAL	-	expression tag	UNP Q8IYV9
B	261	LEU	-	expression tag	UNP Q8IYV9
B	262	PHE	-	expression tag	UNP Q8IYV9
B	263	GLN	-	expression tag	UNP Q8IYV9
C	18	ARG	-	expression tag	UNP Q8IYV9
C	19	SER	-	expression tag	UNP Q8IYV9
C	20	PRO	-	expression tag	UNP Q8IYV9
C	21	TRP	-	expression tag	UNP Q8IYV9
C	256	GLU	-	expression tag	UNP Q8IYV9
C	257	PHE	-	expression tag	UNP Q8IYV9
C	258	LEU	-	expression tag	UNP Q8IYV9
C	259	GLU	-	expression tag	UNP Q8IYV9
C	260	VAL	-	expression tag	UNP Q8IYV9
C	261	LEU	-	expression tag	UNP Q8IYV9
C	262	PHE	-	expression tag	UNP Q8IYV9
C	263	GLN	-	expression tag	UNP Q8IYV9
D	18	ARG	-	expression tag	UNP Q8IYV9
D	19	SER	-	expression tag	UNP Q8IYV9
D	20	PRO	-	expression tag	UNP Q8IYV9
D	21	TRP	-	expression tag	UNP Q8IYV9
D	256	GLU	-	expression tag	UNP Q8IYV9
D	257	PHE	-	expression tag	UNP Q8IYV9
D	258	LEU	-	expression tag	UNP Q8IYV9
D	259	GLU	-	expression tag	UNP Q8IYV9
D	260	VAL	-	expression tag	UNP Q8IYV9
D	261	LEU	-	expression tag	UNP Q8IYV9
D	262	PHE	-	expression tag	UNP Q8IYV9
D	263	GLN	-	expression tag	UNP Q8IYV9
E	18	ARG	-	expression tag	UNP Q8IYV9
E	19	SER	-	expression tag	UNP Q8IYV9
E	20	PRO	-	expression tag	UNP Q8IYV9
E	21	TRP	-	expression tag	UNP Q8IYV9
E	256	GLU	-	expression tag	UNP Q8IYV9
E	257	PHE	-	expression tag	UNP Q8IYV9
E	258	LEU	-	expression tag	UNP Q8IYV9
E	259	GLU	-	expression tag	UNP Q8IYV9
E	260	VAL	-	expression tag	UNP Q8IYV9
E	261	LEU	-	expression tag	UNP Q8IYV9
E	262	PHE	-	expression tag	UNP Q8IYV9

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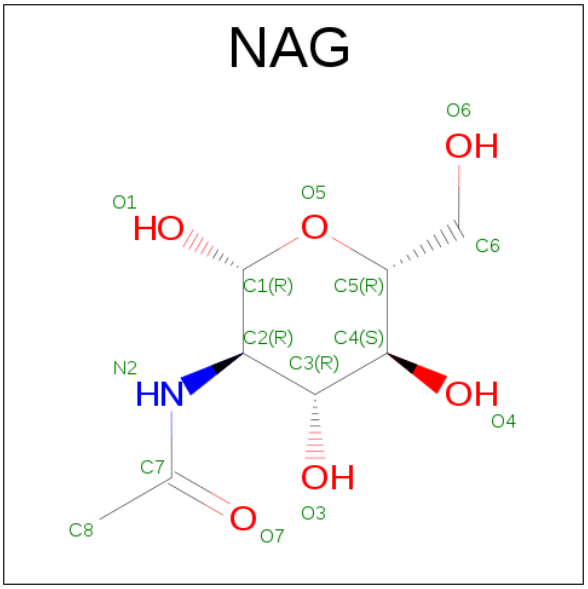
Chain	Residue	Modelled	Actual	Comment	Reference
E	263	GLN	-	expression tag	UNP Q8IYV9
F	18	ARG	-	expression tag	UNP Q8IYV9
F	19	SER	-	expression tag	UNP Q8IYV9
F	20	PRO	-	expression tag	UNP Q8IYV9
F	21	TRP	-	expression tag	UNP Q8IYV9
F	256	GLU	-	expression tag	UNP Q8IYV9
F	257	PHE	-	expression tag	UNP Q8IYV9
F	258	LEU	-	expression tag	UNP Q8IYV9
F	259	GLU	-	expression tag	UNP Q8IYV9
F	260	VAL	-	expression tag	UNP Q8IYV9
F	261	LEU	-	expression tag	UNP Q8IYV9
F	262	PHE	-	expression tag	UNP Q8IYV9
F	263	GLN	-	expression tag	UNP Q8IYV9

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is water.

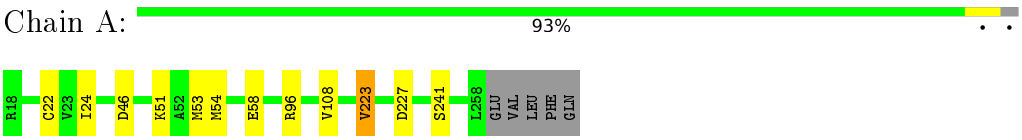
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	132	Total	O	0	0
			132	132		
3	C	78	Total	O	0	0
			78	78		
3	D	65	Total	O	0	0
			65	65		
3	E	39	Total	O	0	0
			39	39		
3	F	57	Total	O	0	0
			57	57		

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.

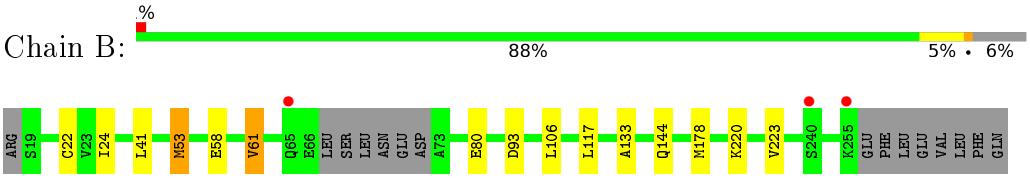
- Molecule 1: Izumo sperm-egg fusion protein 1

Chain A:



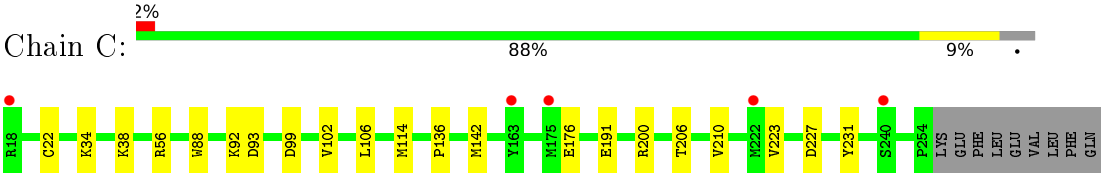
- Molecule 1: Izumo sperm-egg fusion protein 1

Chain B:



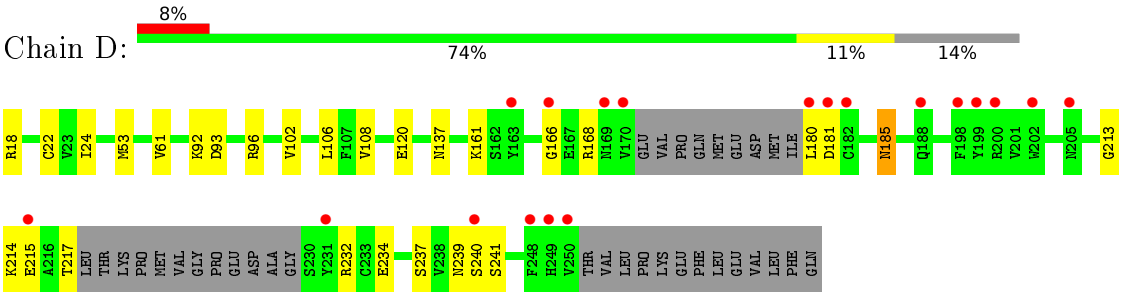
- Molecule 1: Izumo sperm-egg fusion protein 1

Chain C:



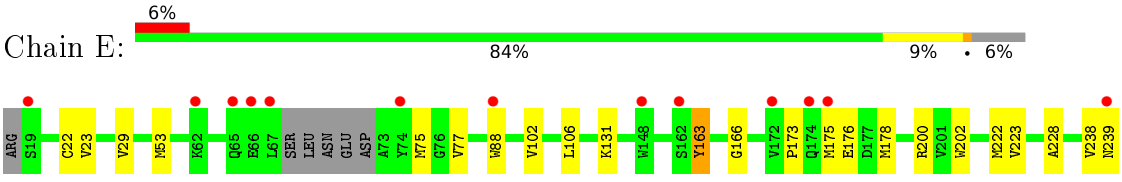
- Molecule 1: Izumo sperm-egg fusion protein 1

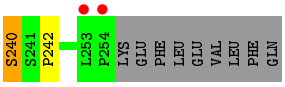
Chain D:



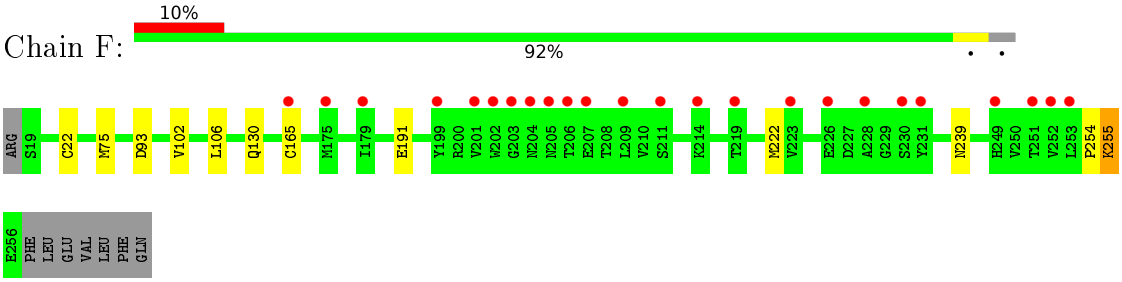
- Molecule 1: Izumo sperm-egg fusion protein 1

Chain E:





• Molecule 1: Izumo sperm-egg fusion protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.94Å 75.07Å 108.89Å 77.65° 79.11° 70.66°	Depositor
Resolution (Å)	50.00 – 2.10 40.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.10) 92.2 (40.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.194 , 0.231 0.200 , 0.236	Depositor DCC
R_{free} test set	5249 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.63	0/1968	0.81	1/2661 (0.0%)
1	B	0.64	0/1880	0.81	0/2541
1	C	0.55	0/1941	0.76	0/2625
1	D	0.60	2/1739 (0.1%)	0.79	1/2346 (0.0%)
1	E	0.53	0/1879	0.74	0/2541
1	F	0.58	0/1937	0.76	0/2620
All	All	0.59	2/11344 (0.0%)	0.78	2/15334 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	GLU	CG-CD	6.08	1.61	1.51
1	D	120	GLU	CB-CG	5.18	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	18	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	1925	0	1885	4	0
1	B	1839	0	1802	8	0
1	C	1896	0	1859	15	0
1	D	1703	0	1657	19	0
1	E	1838	0	1799	15	0
1	F	1895	0	1852	5	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	166	0	0	0	0
3	B	132	0	0	0	0
3	C	78	0	0	1	0
3	D	65	0	0	0	0
3	E	39	0	0	0	0
3	F	57	0	0	0	0
All	All	11717	0	10932	64	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 (64) 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:93:ASP:OD1	1:D:96:ARG:NH1	1.85	1.09
1:B:24:ILE:HG21	1:B:61:VAL:HG13	1.58	0.84
1:D:180:LEU:O	1:D:217:THR:HG22	1.80	0.81
1:D:185:ASN:H	1:D:185:ASN:ND2	1.80	0.78
1:D:24:ILE:HG21	1:D:61:VAL:CG1	2.15	0.77
1:E:173:PRO:HG2	1:E:176:GLU:OE1	1.87	0.73
1:B:24:ILE:HG21	1:B:61:VAL:CG1	2.18	0.73
1:C:34:LYS:O	1:C:38:LYS:HG2	1.89	0.73
1:C:88:TRP:CH2	1:C:92:LYS:HE2	2.28	0.69
1:D:185:ASN:H	1:D:185:ASN:HD22	1.41	0.67
1:D:92:LYS:HE3	1:D:96:ARG:NH2	2.09	0.67
1:C:88:TRP:CZ2	1:C:92:LYS:HE2	2.31	0.65
1:B:41:LEU:HD21	1:B:53:MET:HE1	1.78	0.64
1:B:24:ILE:CG2	1:B:61:VAL:HG13	2.28	0.64
1:C:88:TRP:CH2	1:C:92:LYS:CE	2.81	0.64
1:D:24:ILE:HG21	1:D:61:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:MET:SD	1:E:222:MET:HE2	2.40	0.61
1:E:239:ASN:O	1:E:240:SER:HB2	2.00	0.61
1:A:223:VAL:HG22	1:A:227:ASP:HB2	1.85	0.57
1:E:175:MET:SD	1:E:222:MET:CE	2.93	0.56
1:E:102:VAL:HG23	1:E:106:LEU:HD23	1.88	0.56
1:C:102:VAL:HG23	1:C:106:LEU:HD23	1.86	0.56
1:E:23:VAL:CG1	1:E:29:VAL:HG21	2.36	0.56
1:C:88:TRP:CZ2	1:C:92:LYS:CE	2.89	0.55
1:D:24:ILE:CG2	1:D:61:VAL:CG1	2.84	0.55
1:F:254:PRO:O	1:F:255:LYS:HB2	2.08	0.54
1:A:53:MET:CE	1:A:108:VAL:HG22	2.38	0.52
1:D:168:ARG:NH1	1:D:181:ASP:O	2.43	0.52
1:C:191:GLU:OE1	1:E:88:TRP:HH2	1.93	0.51
1:C:206:THR:HG21	2:C:300:NAG:H82	1.92	0.51
1:C:99:ASP:HB3	1:E:238:VAL:HG12	1.93	0.50
1:B:41:LEU:HD21	1:B:53:MET:CE	2.41	0.50
1:D:237:SER:OG	1:D:239:ASN:HB3	2.11	0.49
1:D:181:ASP:HA	1:D:217:THR:HG22	1.94	0.49
1:D:24:ILE:HD13	1:D:61:VAL:HG12	1.94	0.48
1:F:254:PRO:O	1:F:255:LYS:CB	2.60	0.48
1:D:102:VAL:HG23	1:D:106:LEU:HD23	1.96	0.48
1:D:232:ARG:NH2	1:D:234:GLU:OE2	2.47	0.47
1:E:200:ARG:HG2	1:E:202:TRP:CZ2	2.50	0.47
1:E:238:VAL:HG23	1:E:239:ASN:N	2.29	0.47
1:E:163:TYR:OH	1:E:242:PRO:HD2	2.14	0.47
1:E:178:MET:HB2	1:E:223:VAL:HG11	1.97	0.47
1:D:213:GLY:O	1:D:215:GLU:N	2.48	0.46
1:D:92:LYS:CE	1:D:96:ARG:NH2	2.77	0.46
1:E:200:ARG:NH2	1:E:228:ALA:O	2.49	0.46
1:A:223:VAL:CG2	1:A:227:ASP:HB2	2.46	0.46
1:C:200:ARG:HG3	1:C:210:VAL:HG21	1.97	0.46
1:B:133:ALA:O	1:B:144:GLN:NE2	2.45	0.45
1:F:102:VAL:HG23	1:F:106:LEU:HD23	1.99	0.44
1:D:53:MET:CE	1:D:108:VAL:HG22	2.48	0.43
1:C:223:VAL:HG22	1:C:227:ASP:HB2	1.99	0.43
1:D:137:ASN:O	1:D:161:LYS:HE2	2.19	0.43
1:F:75:MET:H	1:F:130:GLN:HE22	1.67	0.43
1:D:24:ILE:CG2	1:D:61:VAL:HG13	2.50	0.42
1:F:75:MET:H	1:F:130:GLN:NE2	2.18	0.41
1:C:93:ASP:HB3	1:C:114:MET:CG	2.50	0.41
1:E:75:MET:CB	1:E:77:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ARG:HG2	1:C:231:TYR:CE2	2.56	0.41
1:C:136:PRO:HD2	1:C:142:MET:SD	2.61	0.41
1:B:178:MET:HB2	1:B:223:VAL:HG11	2.02	0.41
1:B:24:ILE:CG2	1:B:61:VAL:CG1	2.94	0.41
1:C:56:ARG:NH2	3:C:403:HOH:O	2.54	0.41
1:E:23:VAL:HG12	1:E:29:VAL:HG21	2.00	0.41
1:A:54:MET:O	1:A:58:GLU:HG2	2.20	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	239/246 (97%)	237 (99%)	2 (1%)	0	100	100
1	B	227/246 (92%)	224 (99%)	3 (1%)	0	100	100
1	C	236/246 (96%)	229 (97%)	7 (3%)	0	100	100
1	D	206/246 (84%)	201 (98%)	3 (2%)	2 (1%)	19	13
1	E	227/246 (92%)	218 (96%)	7 (3%)	2 (1%)	21	15
1	F	236/246 (96%)	228 (97%)	7 (3%)	1 (0%)	39	37
All	All	1371/1476 (93%)	1337 (98%)	29 (2%)	5 (0%)	39	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	240	SER
1	D	166	GLY
1	D	214	LYS
1	F	255	LYS
1	E	166	GLY

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	215/220 (98%)	209 (97%)	6 (3%)	51	55
1	B	205/220 (93%)	196 (96%)	9 (4%)	35	33
1	C	212/220 (96%)	210 (99%)	2 (1%)	84	89
1	D	189/220 (86%)	185 (98%)	4 (2%)	61	66
1	E	205/220 (93%)	201 (98%)	4 (2%)	63	68
1	F	212/220 (96%)	206 (97%)	6 (3%)	51	55
All	All	1238/1320 (94%)	1207 (98%)	31 (2%)	55	59

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	24	ILE
1	A	46	ASP
1	A	51	LYS
1	A	223	VAL
1	A	241	SER
1	B	22	CYS
1	B	53	MET
1	B	58	GLU
1	B	61	VAL
1	B	80	GLU
1	B	93	ASP
1	B	106	LEU
1	B	117	LEU
1	B	220	LYS
1	C	22	CYS
1	C	176	GLU
1	D	22	CYS
1	D	185	ASN
1	D	240	SER
1	D	241	SER
1	E	22	CYS

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Mol	Chain	Res	Type
1	E	53	MET
1	E	131	LYS
1	E	163	TYR
1	F	22	CYS
1	F	93	ASP
1	F	165	CYS
1	F	191	GLU
1	F	222	MET
1	F	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	B	130	GLN
1	B	169	ASN
1	B	174	GLN
1	B	247	ASN
1	C	84	GLN
1	C	174	GLN
1	C	185	ASN
1	C	239	ASN
1	D	169	ASN
1	D	185	ASN
1	E	118	GLN
1	F	130	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\|>2$
2	NAG	A	300	1	14,14,15	0.39	0	15,19,21	1.14	1 (6%)
2	NAG	B	300	1	14,14,15	0.43	0	15,19,21	1.06	1 (6%)
2	NAG	C	300	1	14,14,15	0.79	0	15,19,21	1.74	2 (13%)
2	NAG	D	300	1	14,14,15	0.60	0	15,19,21	1.88	2 (13%)
2	NAG	E	300	1	14,14,15	0.65	0	15,19,21	1.05	2 (13%)
2	NAG	F	300	1	14,14,15	0.77	0	15,19,21	1.42	2 (13%)

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
2	NAG	A	300	1	-	0/6/23/26	0/1/1/1
2	NAG	B	300	1	-	0/6/23/26	0/1/1/1
2	NAG	C	300	1	-	0/6/23/26	0/1/1/1
2	NAG	D	300	1	-	0/6/23/26	0/1/1/1
2	NAG	E	300	1	-	0/6/23/26	0/1/1/1
2	NAG	F	300	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	300	NAG	C4-C3-C2	-2.36	107.67	111.34
2	A	300	NAG	O4-C4-C3	-2.27	105.24	110.36
2	E	300	NAG	C4-C3-C2	-2.01	108.22	111.34
2	B	300	NAG	O7-C7-N2	2.02	125.95	121.84
2	F	300	NAG	C2-N2-C7	2.42	126.26	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	300	NAG	C1-O5-C5	2.51	115.83	112.14
2	C	300	NAG	C2-N2-C7	2.71	126.63	123.11
2	F	300	NAG	C1-O5-C5	2.98	116.52	112.14
2	C	300	NAG	C1-O5-C5	5.37	120.03	112.14
2	D	300	NAG	C1-O5-C5	5.99	120.94	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	NAG	1	0

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	241/246 (97%)	0.13	0 100 100	20, 33, 55, 80	0
1	B	231/246 (93%)	-0.00	3 (1%) 79 84	22, 35, 58, 97	0
1	C	237/246 (96%)	0.02	5 (2%) 67 72	29, 43, 67, 96	0
1	D	212/246 (86%)	0.42	19 (8%) 12 16	25, 48, 101, 140	0
1	E	231/246 (93%)	0.37	15 (6%) 22 29	33, 54, 87, 118	0
1	F	238/246 (96%)	0.56	24 (10%) 9 12	29, 52, 92, 125	0
All	All	1390/1476 (94%)	0.25	66 (4%) 35 44	20, 43, 86, 140	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	VAL	6.8
1	F	203	GLY	6.6
1	D	250	VAL	6.4
1	F	205	ASN	5.6
1	F	206	THR	5.6
1	F	199	TYR	5.0
1	D	249	HIS	4.9
1	D	231	TYR	4.8
1	F	253	LEU	4.5
1	E	67	LEU	4.3
1	D	180	LEU	4.1
1	F	204	ASN	3.9
1	D	248	PHE	3.5
1	E	65	GLN	3.5
1	D	163	TYR	3.4
1	D	166	GLY	3.4
1	D	181	ASP	3.3
1	D	169	ASN	3.3
1	D	215	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	226	GLU	3.2
1	F	202	TRP	3.1
1	F	249	HIS	3.0
1	F	201	VAL	3.0
1	F	231	TYR	3.0
1	F	230	SER	3.0
1	E	253	LEU	3.0
1	F	175	MET	2.9
1	D	202	TRP	2.9
1	F	214	LYS	2.9
1	F	251	THR	2.9
1	D	200	ARG	2.8
1	E	19	SER	2.7
1	C	175	MET	2.7
1	C	222	MET	2.7
1	C	18	ARG	2.7
1	C	240	SER	2.6
1	D	188	GLN	2.6
1	F	252	VAL	2.6
1	E	62	LYS	2.5
1	D	182	CYS	2.5
1	B	255	LYS	2.5
1	E	74	TYR	2.5
1	C	163	TYR	2.4
1	D	198	PHE	2.4
1	D	199	TYR	2.4
1	E	162	SER	2.4
1	F	165	CYS	2.3
1	D	205	ASN	2.3
1	E	172	VAL	2.3
1	E	239	ASN	2.3
1	F	211	SER	2.3
1	E	175	MET	2.2
1	F	209	LEU	2.2
1	E	148	TRP	2.2
1	F	207	GLU	2.2
1	B	240	SER	2.2
1	E	66	GLU	2.2
1	B	65	GLN	2.2
1	D	240	SER	2.1
1	F	219	THR	2.1
1	F	179	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	174	GLN	2.1
1	F	228	ALA	2.0
1	E	254	PRO	2.0
1	F	223	VAL	2.0
1	E	88	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	NAG	A	300	14/15	0.88	0.14	0.25	43,53,65,69	0
2	NAG	D	300	14/15	0.88	0.20	-	76,105,111,111	0
2	NAG	B	300	14/15	0.94	0.14	-	43,53,64,66	0
2	NAG	F	300	14/15	0.82	0.39	-	94,108,113,119	0
2	NAG	C	300	14/15	0.82	0.20	-	80,86,95,96	0
2	NAG	E	300	14/15	0.93	0.11	-	73,79,89,93	0

6.5 Other polymers (i)

There are no such residues in this entry.