Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 03:53 PM JST

PDB ID	:	5JKE
Title	:	Crystal structure of human IZUMO1-JUNO complex (crystal form 3)
Authors	:	Ohto, U.; Ishida, H.; Shimizu, T.
Deposited on	:	2016-04-26
Resolution	:	2.86 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

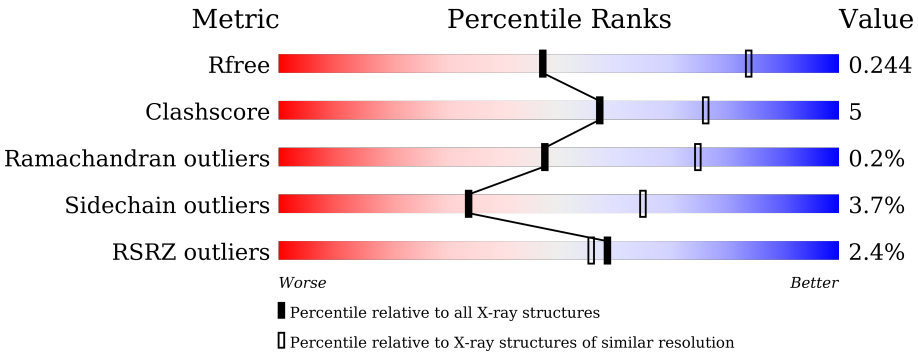
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.86 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	79% 15% • 6%
1	C	246	% 80% 13% • 6%
2	B	221	4% 83% 8% • 8%
2	D	221	5% 81% 10% • 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7066 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	232	Total	C	N	O	S	0	0	0
			1849	1173	312	346	18			
1	C	232	Total	C	N	O	S	0	0	0
			1849	1173	312	346	18			

There are 24 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
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

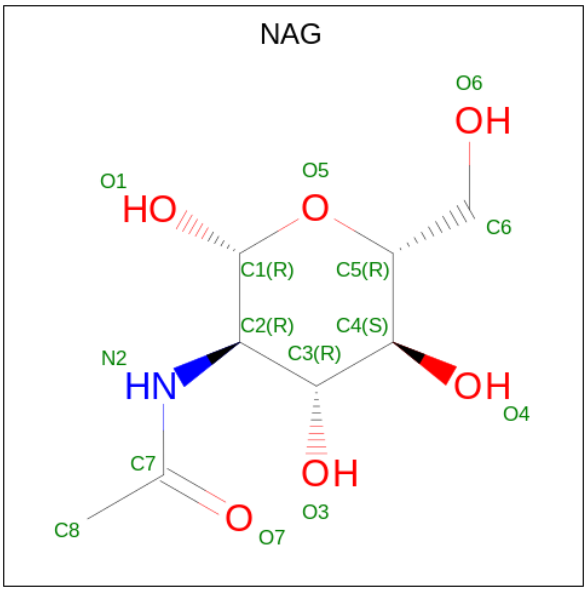
- Molecule 2 is a protein called Sperm-egg fusion protein Juno.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1648	1048	286	295	19			
2	D	203	Total	C	N	O	S	0	0	0
			1648	1048	286	295	19			

There are 24 discrepancies between the modelled and reference sequences:

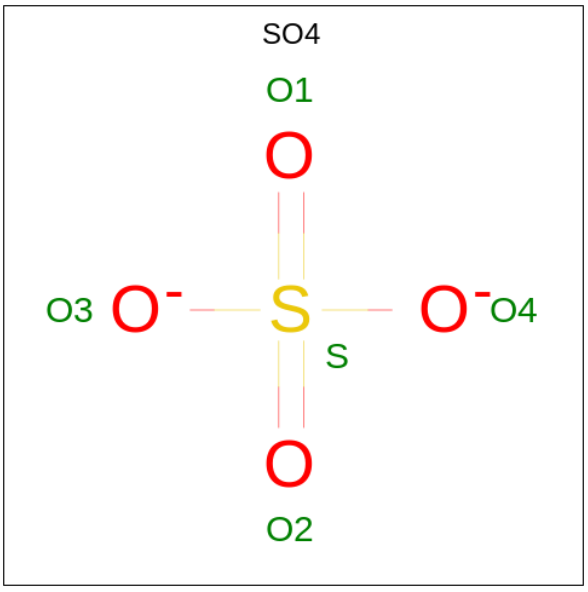
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ARG	-	expression tag	UNP A6ND01
B	17	SER	-	expression tag	UNP A6ND01
B	18	PRO	-	expression tag	UNP A6ND01
B	19	TRP	-	expression tag	UNP A6ND01
B	229	GLU	-	expression tag	UNP A6ND01
B	230	PHE	-	expression tag	UNP A6ND01
B	231	LEU	-	expression tag	UNP A6ND01
B	232	GLU	-	expression tag	UNP A6ND01
B	233	VAL	-	expression tag	UNP A6ND01
B	234	LEU	-	expression tag	UNP A6ND01
B	235	PHE	-	expression tag	UNP A6ND01
B	236	GLN	-	expression tag	UNP A6ND01
D	16	ARG	-	expression tag	UNP A6ND01
D	17	SER	-	expression tag	UNP A6ND01
D	18	PRO	-	expression tag	UNP A6ND01
D	19	TRP	-	expression tag	UNP A6ND01
D	229	GLU	-	expression tag	UNP A6ND01
D	230	PHE	-	expression tag	UNP A6ND01
D	231	LEU	-	expression tag	UNP A6ND01
D	232	GLU	-	expression tag	UNP A6ND01
D	233	VAL	-	expression tag	UNP A6ND01
D	234	LEU	-	expression tag	UNP A6ND01
D	235	PHE	-	expression tag	UNP A6ND01
D	236	GLN	-	expression tag	UNP A6ND01

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

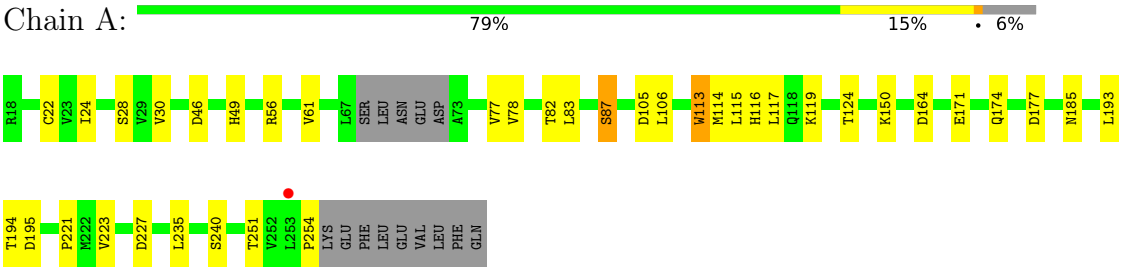
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total O 3 3	0	0
6	D	1	Total O 1 1	0	0

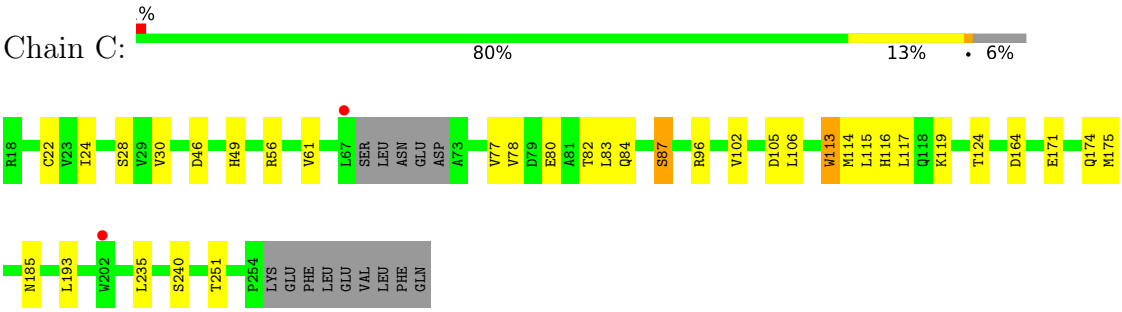
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

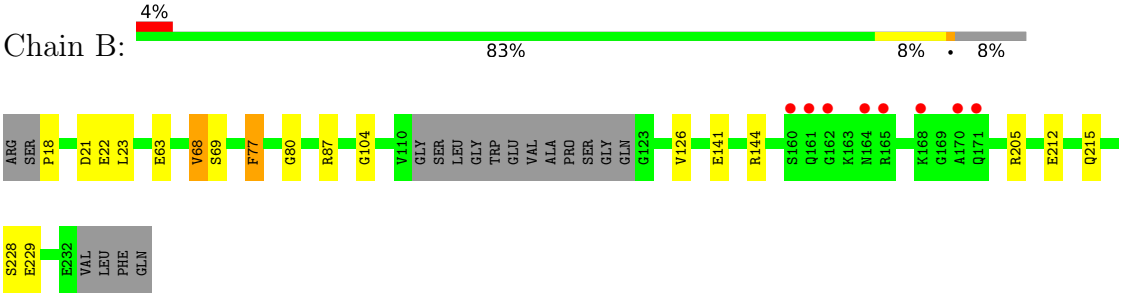
• Molecule 1: Izumo sperm-egg fusion protein 1



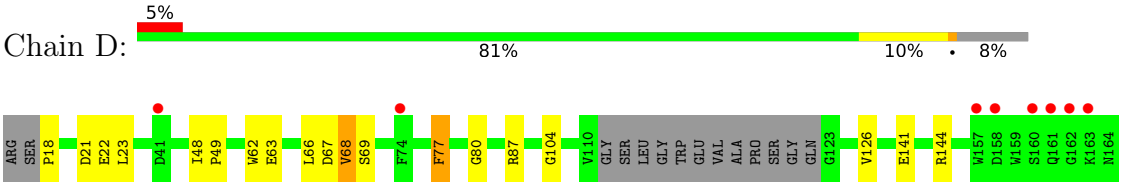
• Molecule 1: Izumo sperm-egg fusion protein 1



• Molecule 2: Sperm-egg fusion protein Juno



• Molecule 2: Sperm-egg fusion protein Juno




R165
A170
E199
R205
E212
Q215
E229
E232
VAL
LEU
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.18Å 141.78Å 144.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.86 45.20 – 2.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.30-2.86) 100.0 (45.20-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.203 , 0.238 0.206 , 0.244	Depositor DCC
R_{free} test set	1468 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	80.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7066	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.92% 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: CL, NAG, SO4

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	0.60	1/1890 (0.1%)	0.80	0/2555
1	C	0.62	1/1890 (0.1%)	0.83	1/2555 (0.0%)
2	B	0.54	0/1706	0.76	2/2320 (0.1%)
2	D	0.53	0/1706	0.76	2/2320 (0.1%)
All	All	0.58	2/7192 (0.0%)	0.79	5/9750 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	TRP	CB-CG	-5.71	1.40	1.50
1	C	113	TRP	CB-CG	-5.37	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	96	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	B	205	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	D	205	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	B	87	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	D	87	ARG	NE-CZ-NH2	-5.09	117.75	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	1849	0	1813	25	0
1	C	1849	0	1813	28	0
2	B	1648	0	1527	7	0
2	D	1648	0	1527	12	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	3	0	0	0	0
6	D	1	0	0	0	0
All	All	7066	0	6732	68	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 5.

All (68) 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:C:102:VAL:HG23	1:C:106:LEU:HD23	1.53	0.89
1:A:177:ASP:OD1	1:A:221:PRO:HA	1.80	0.81
1:C:102:VAL:HG23	1:C:106:LEU:CD2	2.11	0.79
1:C:102:VAL:HG21	1:C:106:LEU:HG	1.65	0.79
2:D:199:GLU:OE1	2:D:205:ARG:NE	2.24	0.70
1:C:102:VAL:CG2	1:C:106:LEU:HG	2.23	0.69
1:C:102:VAL:CG2	1:C:106:LEU:HD23	2.27	0.64
1:C:83:LEU:O	1:C:87:SER:OG	2.16	0.63
1:A:83:LEU:O	1:A:87:SER:OG	2.16	0.63
1:A:177:ASP:OD1	1:A:221:PRO:CA	2.46	0.63
1:C:102:VAL:CG2	1:C:106:LEU:CD2	2.76	0.62
1:A:24:ILE:CG2	1:A:61:VAL:CG1	2.77	0.62
1:A:117:LEU:HB3	1:C:117:LEU:HB3	1.83	0.61
1:C:24:ILE:CG2	1:C:61:VAL:CG1	2.80	0.60
1:A:174:GLN:HE21	1:A:254:PRO:HA	1.68	0.59
1:A:24:ILE:CG2	1:A:61:VAL:HG11	2.33	0.58
1:C:102:VAL:CG2	1:C:106:LEU:CG	2.83	0.57
1:C:24:ILE:CG2	1:C:61:VAL:HG11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:VAL:HG23	2:B:77:PHE:CZ	2.43	0.54
1:C:174:GLN:O	1:C:175:MET:HB2	2.08	0.53
1:A:24:ILE:HG23	1:A:61:VAL:CG1	2.38	0.52
1:C:24:ILE:HG23	1:C:61:VAL:CG1	2.40	0.52
1:A:124:THR:HG21	1:C:124:THR:HB	1.92	0.51
1:A:24:ILE:HG23	1:A:61:VAL:HG13	1.93	0.50
2:D:68:VAL:HG23	2:D:77:PHE:CZ	2.46	0.50
1:A:24:ILE:HG21	1:A:61:VAL:CG1	2.40	0.50
1:C:80:GLU:OE2	1:C:84:GLN:OE1	2.29	0.49
1:A:114:MET:HB2	1:C:113:TRP:HE1	1.78	0.49
1:A:113:TRP:HE1	1:C:114:MET:HB2	1.77	0.49
1:C:24:ILE:HG23	1:C:61:VAL:HG13	1.95	0.48
2:B:63:GLU:O	2:B:69:SER:OG	2.25	0.48
1:C:24:ILE:HG21	1:C:61:VAL:CG1	2.43	0.47
2:D:63:GLU:O	2:D:69:SER:OG	2.25	0.47
2:B:18:PRO:O	2:B:229:GLU:HG3	2.15	0.47
1:A:174:GLN:NE2	1:A:254:PRO:HA	2.30	0.46
2:D:18:PRO:O	2:D:229:GLU:HG3	2.15	0.46
1:A:24:ILE:HG21	1:A:61:VAL:HG11	1.98	0.45
2:B:212:GLU:HB3	2:B:215:GLN:HG2	1.99	0.44
1:A:116:HIS:HD2	1:A:117:LEU:HD22	1.82	0.44
2:B:77:PHE:O	2:B:80:GLY:N	2.48	0.44
2:D:77:PHE:O	2:D:80:GLY:N	2.50	0.44
2:D:212:GLU:HB3	2:D:215:GLN:HG2	2.00	0.44
2:B:23:LEU:O	2:B:104:GLY:HA3	2.18	0.44
1:A:116:HIS:CD2	1:A:117:LEU:HD22	2.53	0.43
1:C:46:ASP:HB2	1:C:49:HIS:HD2	1.83	0.43
2:D:141:GLU:OE2	2:D:144:ARG:NH2	2.46	0.43
2:D:199:GLU:OE1	2:D:205:ARG:CZ	2.67	0.43
2:B:141:GLU:OE2	2:B:144:ARG:NH2	2.48	0.43
1:C:24:ILE:HG21	1:C:61:VAL:HG11	2.00	0.43
1:C:115:LEU:O	1:C:119:LYS:HG3	2.19	0.43
1:C:116:HIS:CD2	1:C:117:LEU:HD22	2.54	0.43
1:A:193:LEU:HD13	1:A:235:LEU:HD21	1.99	0.42
1:C:171:GLU:HG2	1:C:251:THR:HB	2.01	0.42
2:D:23:LEU:O	2:D:104:GLY:HA3	2.19	0.42
1:C:77:VAL:O	1:C:78:VAL:HG23	2.20	0.42
1:A:77:VAL:O	1:A:78:VAL:HG23	2.19	0.42
1:C:78:VAL:HG13	1:C:82:THR:HB	2.01	0.42
1:C:116:HIS:HD2	1:C:117:LEU:HD22	1.85	0.42
1:C:193:LEU:HD13	1:C:235:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ILE:N	2:D:49:PRO:CD	2.83	0.42
1:A:171:GLU:HG2	1:A:251:THR:HB	2.01	0.42
1:A:115:LEU:O	1:A:119:LYS:HG3	2.19	0.41
1:A:78:VAL:HG13	1:A:82:THR:HB	2.00	0.41
2:D:62:TRP:CZ2	2:D:66:LEU:HD21	2.55	0.41
1:A:46:ASP:HB2	1:A:49:HIS:HD2	1.86	0.41
1:A:194:THR:OG1	1:A:195:ASP:N	2.53	0.40
1:A:223:VAL:CG2	1:A:227:ASP:HB2	2.50	0.40
2:D:67:ASP:HB3	2:D:77:PHE:CZ	2.57	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	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
1	C	228/246 (93%)	222 (97%)	6 (3%)	0	100	100
2	B	199/221 (90%)	191 (96%)	7 (4%)	1 (0%)	29	57
2	D	199/221 (90%)	190 (96%)	8 (4%)	1 (0%)	29	57
All	All	854/934 (91%)	824 (96%)	28 (3%)	2 (0%)	47	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	68	VAL
2	D	68	VAL

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	206/220 (94%)	195 (95%)	11 (5%)	22 50
1	C	206/220 (94%)	197 (96%)	9 (4%)	28 58
2	B	181/195 (93%)	176 (97%)	5 (3%)	43 73
2	D	181/195 (93%)	177 (98%)	4 (2%)	52 79
All	All	774/830 (93%)	745 (96%)	29 (4%)	34 65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	28	SER
1	A	30	VAL
1	A	56	ARG
1	A	87	SER
1	A	105	ASP
1	A	106	LEU
1	A	150	LYS
1	A	164	ASP
1	A	185	ASN
1	A	240	SER
2	B	21	ASP
2	B	22	GLU
2	B	77	PHE
2	B	126	VAL
2	B	228	SER
1	C	22	CYS
1	C	28	SER
1	C	30	VAL
1	C	56	ARG
1	C	87	SER
1	C	105	ASP
1	C	164	ASP
1	C	185	ASN

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Mol	Chain	Res	Type
1	C	240	SER
2	D	21	ASP
2	D	22	GLU
2	D	77	PHE
2	D	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	84	GLN
1	A	118	GLN
1	A	174	GLN
1	A	239	ASN
1	C	49	HIS
1	C	84	GLN
1	C	118	GLN
1	C	174	GLN
1	C	239	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	NAG	C	300	1	14,14,15	0.80	0	17,19,21	1.60	2 (11%)
3	NAG	A	301	1	14,14,15	0.89	1 (7%)	17,19,21	2.87	5 (29%)
3	NAG	D	301	2	14,14,15	0.80	1 (7%)	17,19,21	1.82	6 (35%)
4	SO4	A	302	-	4,4,4	0.39	0	6,6,6	0.15	0
4	SO4	D	302	-	4,4,4	0.45	0	6,6,6	0.29	0
3	NAG	B	301	2	14,14,15	0.87	1 (7%)	17,19,21	1.70	5 (29%)

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	C	300	1	-	2/6/23/26	0/1/1/1
3	NAG	A	301	1	-	2/6/23/26	0/1/1/1
3	NAG	D	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	C1-C2	2.43	1.56	1.52
3	A	301	NAG	C1-C2	2.36	1.55	1.52
3	D	301	NAG	C1-C2	2.03	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	NAG	C1-O5-C5	10.03	125.78	112.19
3	C	300	NAG	O5-C5-C6	4.25	113.87	107.20
3	B	301	NAG	O5-C5-C6	3.47	112.65	107.20
3	D	301	NAG	O5-C5-C6	3.43	112.58	107.20
3	A	301	NAG	O5-C5-C6	2.86	111.69	107.20
3	A	301	NAG	C2-N2-C7	2.86	126.97	122.90
3	A	301	NAG	C4-C3-C2	2.76	115.07	111.02
3	D	301	NAG	O4-C4-C5	2.66	115.89	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	NAG	O5-C5-C4	-2.60	104.49	110.83
3	B	301	NAG	C4-C3-C2	2.58	114.79	111.02
3	D	301	NAG	C3-C4-C5	-2.53	105.72	110.24
3	D	301	NAG	O5-C5-C4	-2.52	104.69	110.83
3	A	301	NAG	O5-C1-C2	2.43	115.12	111.29
3	C	300	NAG	C1-C2-N2	2.41	114.60	110.49
3	D	301	NAG	C1-C2-N2	-2.27	106.61	110.49
3	D	301	NAG	C2-N2-C7	2.15	125.97	122.90
3	B	301	NAG	C2-N2-C7	2.04	125.81	122.90
3	B	301	NAG	O4-C4-C5	2.01	114.28	109.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NAG	C4-C5-C6-O6
3	A	301	NAG	O5-C5-C6-O6
3	C	300	NAG	C4-C5-C6-O6
3	C	300	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	232/246 (94%)	0.11	1 (0%)	92	92	47, 81, 123, 149	0
1	C	232/246 (94%)	0.18	2 (0%)	84	84	46, 88, 125, 143	0
2	B	203/221 (91%)	0.20	8 (3%)	39	34	50, 83, 125, 161	0
2	D	203/221 (91%)	0.23	10 (4%)	29	25	50, 83, 133, 173	0
All	All	870/934 (93%)	0.18	21 (2%)	59	56	46, 83, 126, 173	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	162	GLY	4.8
2	D	160	SER	4.4
2	B	168	LYS	4.2
2	D	157	TRP	3.7
2	D	162	GLY	3.4
2	B	160	SER	3.2
2	D	170	ALA	3.1
2	D	161	GLN	2.9
2	D	158	ASP	2.9
1	C	67	LEU	2.8
2	B	170	ALA	2.8
2	D	163	LYS	2.6
2	B	171	GLN	2.6
2	B	164	ASN	2.4
2	B	165	ARG	2.4
2	D	74	PHE	2.4
1	C	202	TRP	2.3
2	D	41	ASP	2.2
1	A	253	LEU	2.2
2	B	161	GLN	2.2
2	D	165	ARG	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	NAG	B	301	14/15	0.69	0.35	125,150,157,158	0
3	NAG	D	301	14/15	0.75	0.30	115,129,139,143	0
3	NAG	A	301	14/15	0.76	0.34	118,133,146,146	0
4	SO4	D	302	5/5	0.76	0.32	88,114,160,161	0
3	NAG	C	300	14/15	0.83	0.45	108,132,161,162	0
4	SO4	A	302	5/5	0.90	0.57	116,117,127,132	0
5	CL	D	303	1/1	0.95	0.14	62,62,62,62	0
5	CL	B	302	1/1	0.97	0.14	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.