



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:39 AM GMT

PDB ID : 3O4O
Title : Crystal structure of an Interleukin-1 receptor complex
Authors : Wang, X.Q.; Wang, D.L.; Zhang, S.Y.; Li, L.; Liu, X.; Mei, K.R.
Deposited on : 2010-07-27
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

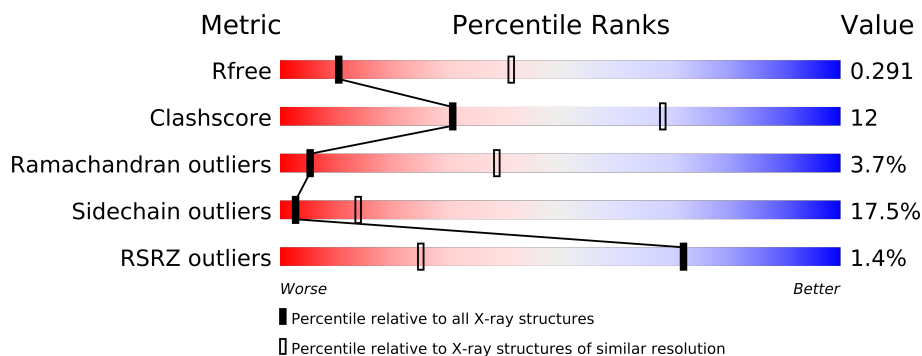
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	158	
2	C	339	
3	B	339	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	B	337	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6506 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Interleukin-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1212	770	200	234	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P01584
A	-3	PRO	-	EXPRESSION TAG	UNP P01584
A	-2	LEU	-	EXPRESSION TAG	UNP P01584
A	-1	GLY	-	EXPRESSION TAG	UNP P01584
A	0	SER	-	EXPRESSION TAG	UNP P01584

- Molecule 2 is a protein called Interleukin-1 receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	316	2562	1631	439	480	12	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	EXPRESSION TAG	UNP P27930
C	-1	ASP	-	EXPRESSION TAG	UNP P27930
C	0	PRO	-	EXPRESSION TAG	UNP P27930
C	331	HIS	-	EXPRESSION TAG	UNP P27930
C	332	HIS	-	EXPRESSION TAG	UNP P27930
C	333	HIS	-	EXPRESSION TAG	UNP P27930
C	334	HIS	-	EXPRESSION TAG	UNP P27930
C	335	HIS	-	EXPRESSION TAG	UNP P27930
C	336	HIS	-	EXPRESSION TAG	UNP P27930

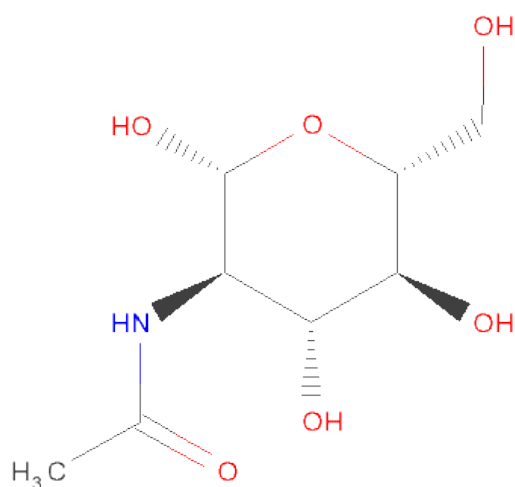
- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	323	Total	C	N	O	S	0	0	0
			2620	1673	442	489	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	EXPRESSION TAG	UNP Q9NPH3
B	-1	ASP	-	EXPRESSION TAG	UNP Q9NPH3
B	0	PRO	-	EXPRESSION TAG	UNP Q9NPH3
B	331	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	332	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	333	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	334	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	335	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	336	HIS	-	EXPRESSION TAG	UNP Q9NPH3

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

There are 18 discrepancies between the modelled and reference sequences:

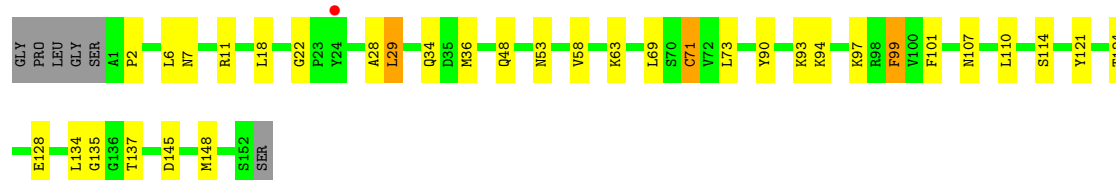
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	EXPRESSION TAG	UNP Q9NPH3
B	-1	ASP	-	EXPRESSION TAG	UNP Q9NPH3
B	0	PRO	-	EXPRESSION TAG	UNP Q9NPH3
B	331	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	332	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	333	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	334	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	335	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	336	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	-2	ALA	-	EXPRESSION TAG	UNP Q9NPH3
B	-1	ASP	-	EXPRESSION TAG	UNP Q9NPH3
B	0	PRO	-	EXPRESSION TAG	UNP Q9NPH3
B	331	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	332	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	333	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	334	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	335	HIS	-	EXPRESSION TAG	UNP Q9NPH3
B	336	HIS	-	EXPRESSION TAG	UNP Q9NPH3

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.

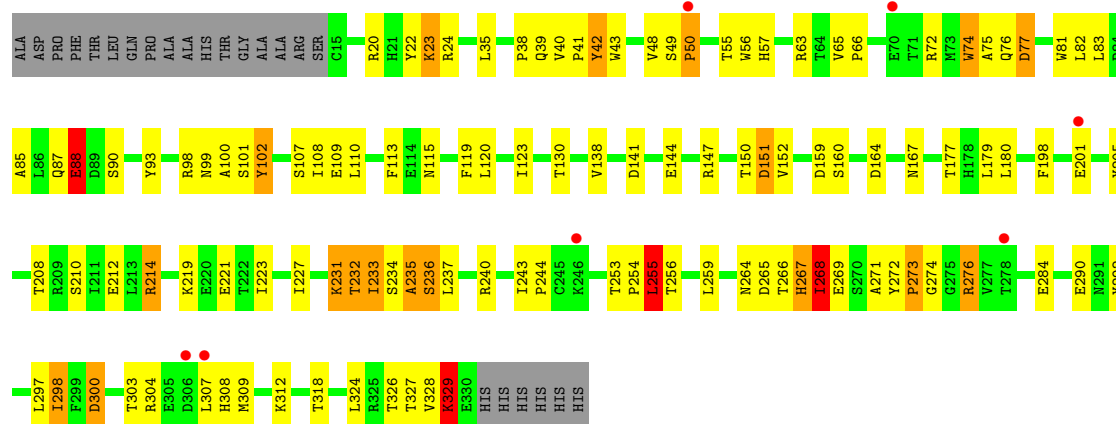
- Molecule 1: Interleukin-1 beta

Chain A: 



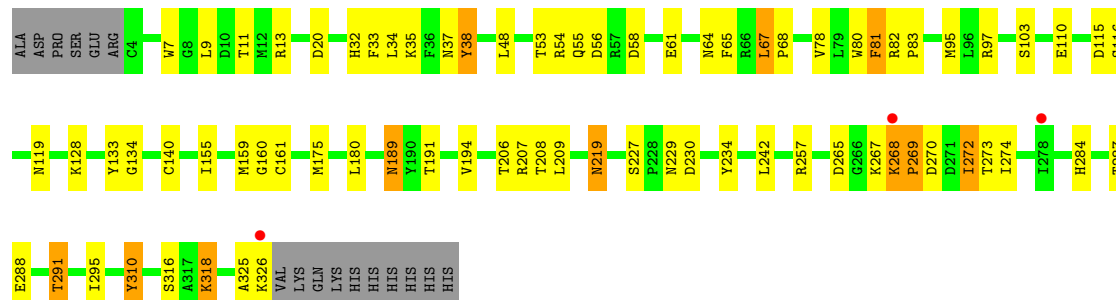
- Molecule 2: Interleukin-1 receptor type 2

Chain C: 



- Molecule 3: Interleukin-1 receptor accessory protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.83Å 177.47Å 180.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.59 – 3.30 36.58 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (36.59-3.30) 94.8 (36.58-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.252 , 0.289 0.247 , 0.291	Depositor DCC
R_{free} test set	1100 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.5	EDS
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 21444 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.42	0/1235	0.54	0/1662
2	C	0.29	0/2626	0.53	0/3573
3	B	0.33	0/2689	0.52	0/3659
All	All	0.34	0/6550	0.53	0/8894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1212	0	0	10	0
2	C	2562	0	0	45	0
3	B	2620	0	0	23	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
5	B	56	0	0	1	0
All	All	6506	0	0	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 12.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:99:ASN:O	2:C:102:TYR:N	1.99	0.94
3:B:55:GLN:CA	5:B:338:NAG:O7	2.38	0.72
1:A:58:VAL:N	1:A:101:PHE:O	2.24	0.71
3:B:234:TYR:O	3:B:326:LYS:CA	2.45	0.64
2:C:82:LEU:O	2:C:85:ALA:N	2.32	0.63
3:B:234:TYR:O	3:B:325:ALA:O	2.17	0.62
3:B:67:LEU:N	3:B:68:PRO:CA	2.64	0.61
2:C:102:TYR:CD2	2:C:102:TYR:C	2.73	0.61
2:C:327:THR:CG2	2:C:328:VAL:N	2.66	0.59
3:B:81:PHE:CD1	3:B:81:PHE:N	2.71	0.58
3:B:267:LYS:O	3:B:268:LYS:C	2.43	0.57
2:C:65:VAL:N	2:C:66:PRO:CA	2.68	0.57
2:C:214:ARG:CG	2:C:214:ARG:NH1	2.68	0.56
1:A:28:ALA:O	1:A:128:GLU:O	2.24	0.56
2:C:74:TRP:CD1	2:C:75:ALA:N	2.74	0.55
2:C:87:GLN:O	2:C:88:GLU:CB	2.56	0.54
3:B:268:LYS:O	3:B:269:PRO:O	2.25	0.54
1:A:99:PHE:N	1:A:99:PHE:CD2	2.77	0.52
2:C:159:ASP:O	2:C:160:SER:OG	2.28	0.51
3:B:219:ASN:OD1	3:B:219:ASN:N	2.44	0.51
2:C:99:ASN:O	2:C:102:TYR:O	2.28	0.50
2:C:266:THR:O	2:C:267:HIS:CB	2.60	0.50
2:C:274:GLY:N	2:C:276:ARG:NH1	2.59	0.50
2:C:81:TRP:N	2:C:81:TRP:CD1	2.79	0.50
2:C:49:SER:O	2:C:50:PRO:C	2.50	0.50
1:A:94:LYS:N	1:A:94:LYS:CD	2.75	0.50
2:C:38:PRO:O	2:C:40:VAL:N	2.45	0.49
2:C:147:ARG:CG	2:C:147:ARG:NH1	2.74	0.49
2:C:164:ASP:O	2:C:167:ASN:N	2.46	0.49
2:C:328:VAL:O	2:C:329:LYS:CB	2.60	0.49
2:C:22:TYR:CD1	2:C:23:LYS:N	2.82	0.47
2:C:99:ASN:O	2:C:100:ALA:C	2.53	0.47
2:C:99:ASN:O	2:C:101:SER:N	2.47	0.47
2:C:227:ILE:O	2:C:227:ILE:CG2	2.63	0.47
3:B:115:ASP:OD1	3:B:116:SER:N	2.48	0.47
2:C:272:TYR:N	2:C:273:PRO:CD	2.79	0.46
3:B:291:THR:OG1	3:B:291:THR:O	2.34	0.46
2:C:312:LYS:CA	2:C:324:LEU:O	2.63	0.46
2:C:198:PHE:N	2:C:205:TYR:O	2.49	0.45
2:C:93:TYR:O	2:C:107:SER:CA	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:42:TYR:N	2:C:42:TYR:CD2	2.84	0.45
3:B:64:ASN:OD1	3:B:64:ASN:C	2.55	0.45
3:B:310:TYR:CD2	3:B:310:TYR:N	2.84	0.45
3:B:189:ASN:ND2	3:B:189:ASN:N	2.64	0.45
3:B:37:ASN:O	3:B:38:TYR:CB	2.64	0.44
2:C:93:TYR:CD1	2:C:93:TYR:N	2.86	0.44
3:B:316:SER:C	3:B:318:LYS:N	2.70	0.44
1:A:29:LEU:CD2	1:A:29:LEU:N	2.81	0.44
3:B:54:ARG:CG	3:B:55:GLN:N	2.81	0.44
2:C:236:SER:O	2:C:237:LEU:CB	2.66	0.44
1:A:121:TYR:N	1:A:135:GLY:O	2.51	0.44
1:A:121:TYR:O	1:A:135:GLY:N	2.50	0.43
3:B:274:ILE:CG2	3:B:274:ILE:O	2.64	0.43
2:C:268:ILE:CG2	2:C:268:ILE:O	2.65	0.43
2:C:99:ASN:C	2:C:101:SER:N	2.69	0.43
3:B:115:ASP:OD2	3:B:119:ASN:ND2	2.51	0.43
2:C:113:PHE:CD2	2:C:119:PHE:CD1	3.07	0.43
2:C:123:ILE:CG2	2:C:123:ILE:O	2.67	0.43
3:B:95:MET:CA	3:B:103:SER:O	2.67	0.42
2:C:109:GLU:CG	2:C:110:LEU:N	2.82	0.42
3:B:7:TRP:CZ2	3:B:32:HIS:CD2	3.07	0.42
2:C:123:ILE:N	2:C:123:ILE:CD1	2.83	0.42
1:A:34:GLN:O	2:C:24:ARG:NH2	2.53	0.42
2:C:76:GLN:CB	2:C:81:TRP:NE1	2.82	0.42
3:B:229:ASN:O	3:B:230:ASP:CB	2.68	0.41
2:C:243:ILE:CG2	2:C:298:ILE:CG2	2.98	0.41
2:C:265:ASP:OD2	2:C:265:ASP:N	2.53	0.41
1:A:71:CYS:SG	1:A:114:SER:OG	2.78	0.41
2:C:231:LYS:O	2:C:233:ILE:N	2.54	0.41
2:C:255:LEU:CG	2:C:256:THR:N	2.84	0.41
3:B:134:GLY:O	3:B:180:LEU:O	2.38	0.41
1:A:90:TYR:N	1:A:90:TYR:CD1	2.89	0.41
2:C:300:ASP:OD2	2:C:300:ASP:N	2.54	0.41
2:C:243:ILE:O	2:C:243:ILE:CG2	2.69	0.41
2:C:253:THR:N	2:C:254:PRO:CD	2.84	0.41
2:C:234:SER:O	2:C:235:ALA:CB	2.69	0.41
3:B:287:THR:O	3:B:288:GLU:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/158 (95%)	134 (89%)	14 (9%)	2 (1%)	18	69
2	C	314/339 (93%)	254 (81%)	41 (13%)	19 (6%)	2	22
3	B	321/339 (95%)	271 (84%)	42 (13%)	8 (2%)	9	51
All	All	785/836 (94%)	659 (84%)	97 (12%)	29 (4%)	5	39

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
2	C	50	PRO
2	C	236	SER
2	C	244	PRO
2	C	264	ASN
2	C	268	ILE
2	C	329	LYS
3	B	38	TYR
3	B	265	ASP
3	B	269	PRO
2	C	151	ASP
2	C	152	VAL
2	C	232	THR
2	C	235	ALA
3	B	272	ILE
2	C	39	GLN
2	C	77	ASP
2	C	88	GLU
2	C	150	THR
2	C	255	LEU
2	C	271	ALA
3	B	273	THR
2	C	273	PRO
3	B	159	MET
3	B	268	LYS

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Mol	Chain	Res	Type
2	C	141	ASP
1	A	22	GLY
2	C	41	PRO
3	B	160	GLY

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	139/143 (97%)	117 (84%)	22 (16%)	4	18
2	C	287/304 (94%)	227 (79%)	60 (21%)	1	8
3	B	299/314 (95%)	254 (85%)	45 (15%)	4	21
All	All	725/761 (95%)	598 (82%)	127 (18%)	3	14

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	ASN
1	A	11	ARG
1	A	18	LEU
1	A	29	LEU
1	A	36	MET
1	A	48	GLN
1	A	53	ASN
1	A	63	LYS
1	A	69	LEU
1	A	71	CYS
1	A	73	LEU
1	A	93	LYS
1	A	97	LYS
1	A	99	PHE
1	A	107	ASN
1	A	110	LEU
1	A	124	THR
1	A	134	LEU

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Mol	Chain	Res	Type
1	A	137	THR
1	A	145	ASP
1	A	148	MET
2	C	20	ARG
2	C	23	LYS
2	C	35	LEU
2	C	42	TYR
2	C	43	TRP
2	C	48	VAL
2	C	55	THR
2	C	56	TRP
2	C	57	HIS
2	C	63	ARG
2	C	72	ARG
2	C	74	TRP
2	C	77	ASP
2	C	83	LEU
2	C	88	GLU
2	C	90	SER
2	C	98	ARG
2	C	102	TYR
2	C	108	ILE
2	C	115	ASN
2	C	120	LEU
2	C	130	THR
2	C	138	VAL
2	C	144	GLU
2	C	151	ASP
2	C	177	THR
2	C	179	LEU
2	C	180	LEU
2	C	201	GLU
2	C	208	THR
2	C	210	SER
2	C	212	GLU
2	C	214	ARG
2	C	219	LYS
2	C	221	GLU
2	C	223	ILE
2	C	231	LYS
2	C	232	THR
2	C	233	ILE

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Mol	Chain	Res	Type
2	C	240	ARG
2	C	255	LEU
2	C	259	LEU
2	C	267	HIS
2	C	268	ILE
2	C	269	GLU
2	C	276	ARG
2	C	284	GLU
2	C	290	GLU
2	C	292	TYR
2	C	297	LEU
2	C	298	ILE
2	C	300	ASP
2	C	303	THR
2	C	304	ARG
2	C	307	LEU
2	C	308	HIS
2	C	309	MET
2	C	318	THR
2	C	326	THR
2	C	329	LYS
3	B	9	LEU
3	B	11	THR
3	B	13	ARG
3	B	20	ASP
3	B	33	PHE
3	B	34	LEU
3	B	35	LYS
3	B	48	LEU
3	B	53	THR
3	B	56	ASP
3	B	58	ASP
3	B	61	GLU
3	B	65	PHE
3	B	67	LEU
3	B	78	VAL
3	B	80	TRP
3	B	81	PHE
3	B	82	ARG
3	B	83	PRO
3	B	97	ARG
3	B	110	GLU

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Mol	Chain	Res	Type
3	B	128	LYS
3	B	133	TYR
3	B	140	CYS
3	B	155	ILE
3	B	161	CYS
3	B	175	MET
3	B	189	ASN
3	B	191	THR
3	B	194	VAL
3	B	206	THR
3	B	207	ARG
3	B	208	THR
3	B	209	LEU
3	B	219	ASN
3	B	227	SER
3	B	242	LEU
3	B	257	ARG
3	B	270	ASP
3	B	272	ILE
3	B	284	HIS
3	B	291	THR
3	B	295	ILE
3	B	310	TYR
3	B	318	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	$\# Z > 2$
5	NAG	B	338	3,5	12,14,15	0.87	1 (8%)	15,19,21	1.71	3 (20%)
5	NAG	B	339	5	12,14,15	0.69	0	15,19,21	1.31	2 (13%)
5	NAG	B	341	3,5	12,14,15	0.66	1 (8%)	15,19,21	0.88	1 (6%)
5	NAG	B	342	5	12,14,15	0.66	0	15,19,21	1.01	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
5	NAG	B	338	3,5	-	0/6/23/26	0/1/1/1
5	NAG	B	339	5	-	0/6/23/26	0/1/1/1
5	NAG	B	341	3,5	-	0/6/23/26	0/1/1/1
5	NAG	B	342	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	338	NAG	O5-C5	-2.70	1.40	1.45
5	B	341	NAG	O5-C5	-2.08	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	338	NAG	C2-N2-C7	-4.05	116.29	123.09
5	B	339	NAG	C2-N2-C7	-3.11	117.87	123.09
5	B	342	NAG	O5-C5-C6	2.63	109.74	106.98
5	B	339	NAG	C3-C2-N2	-2.52	107.93	111.76
5	B	338	NAG	O4-C4-C5	2.51	115.90	109.28
5	B	338	NAG	C3-C2-N2	-2.31	108.25	111.76
5	B	341	NAG	C3-C2-N2	-2.21	108.40	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	B	337	3	12,14,15	0.69	1 (8%)	15,19,21	0.99	2 (13%)
4	NAG	B	340	3	12,14,15	0.82	1 (8%)	15,19,21	1.08	1 (6%)
4	NAG	C	337	2	12,14,15	0.87	1 (8%)	15,19,21	1.35	3 (20%)
4	NAG	C	338	2	12,14,15	0.62	0	15,19,21	1.08	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	B	337	3	-	0/6/23/26	0/1/1/1
4	NAG	B	340	3	-	2/6/23/26	0/1/1/1
4	NAG	C	337	2	-	0/6/23/26	0/1/1/1
4	NAG	C	338	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)
4	B	340	NAG	O5-C5	-2.39	1.41	1.45
4	B	337	NAG	O5-C5	-2.13	1.41	1.45
4	C	337	NAG	C2-N2	-2.05	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	337	NAG	O5-C5-C6	3.71	110.87	106.98
4	B	340	NAG	C2-N2-C7	-3.06	117.94	123.09
4	C	338	NAG	O5-C5-C6	2.75	109.87	106.98
4	B	337	NAG	O5-C5-C6	2.65	109.76	106.98
4	C	337	NAG	C2-N2-C7	-2.17	119.45	123.09
4	C	337	NAG	C3-C2-N2	-2.16	108.48	111.76
4	B	337	NAG	C3-C2-N2	-2.11	108.55	111.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	340	NAG	C8-C7-N2-C2
4	B	340	NAG	O7-C7-N2-C2

There are no ring outliers.

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, 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	152/158 (96%)	-0.06	1 (0%)	84 42	53, 99, 166, 210	0
2	C	316/339 (93%)	0.18	7 (2%)	59 16	54, 139, 207, 253	0
3	B	323/339 (95%)	0.09	3 (0%)	81 37	46, 118, 199, 231	0
All	All	791/836 (94%)	0.10	11 (1%)	72 25	46, 122, 202, 253	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	268	LYS	3.8
1	A	24	TYR	2.9
2	C	50	PRO	2.8
2	C	70	GLU	2.8
2	C	278	THR	2.4
2	C	306	ASP	2.4
2	C	307	LEU	2.3
3	B	278	ILE	2.3
2	C	201	GLU	2.2
3	B	326	LYS	2.2
2	C	246	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	341	14/15	0.20	0.36	116,118,120,122	0
5	NAG	B	338	14/15	0.17	-0.78	148,154,159,161	0
5	NAG	B	339	14/15	0.20	-8.28	142,148,154,155	0
5	NAG	B	342	14/15	0.28	-	114,118,119,121	0

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	337	14/15	0.29	7.16	182,187,191,192	0
4	NAG	B	340	14/15	0.25	-0.07	154,162,170,173	0
4	NAG	C	337	14/15	0.20	-0.72	151,160,169,169	0
4	NAG	C	338	14/15	0.14	-1.32	127,136,142,145	0

6.5 Other polymers

There are no such residues in this entry.