



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 PM GMT

PDB ID : 4R6U
Title : IL-18 receptor complex
Authors : Wei, H.; Wang, X.
Deposited on : 2014-08-26
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

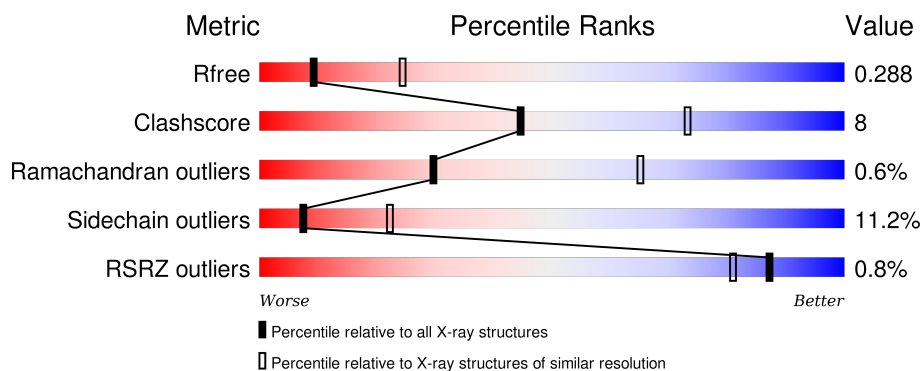
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>23%</div> <div>5%</div> <div>14%</div> </div> </div>
1	C	317	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>23%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	157	<div> <div></div> <div> <div>83%</div> <div>14%</div> <div>••</div> </div> </div>
2	D	157	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	402	-	-	-	X
3	NAG	A	403	-	-	-	X
3	NAG	C	803	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7101 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 Interleukin-18 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	275	Total	C	N	O	S	0	0	0
			2241	1425	388	414	14			
1	A	274	Total	C	N	O	S	0	0	0
			2234	1421	387	412	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	330	HIS	-	EXPRESSION TAG	UNP Q13478
C	331	HIS	-	EXPRESSION TAG	UNP Q13478
C	332	HIS	-	EXPRESSION TAG	UNP Q13478
C	333	HIS	-	EXPRESSION TAG	UNP Q13478
C	334	HIS	-	EXPRESSION TAG	UNP Q13478
C	335	HIS	-	EXPRESSION TAG	UNP Q13478
A	330	HIS	-	EXPRESSION TAG	UNP Q13478
A	331	HIS	-	EXPRESSION TAG	UNP Q13478
A	332	HIS	-	EXPRESSION TAG	UNP Q13478
A	333	HIS	-	EXPRESSION TAG	UNP Q13478
A	334	HIS	-	EXPRESSION TAG	UNP Q13478
A	335	HIS	-	EXPRESSION TAG	UNP Q13478

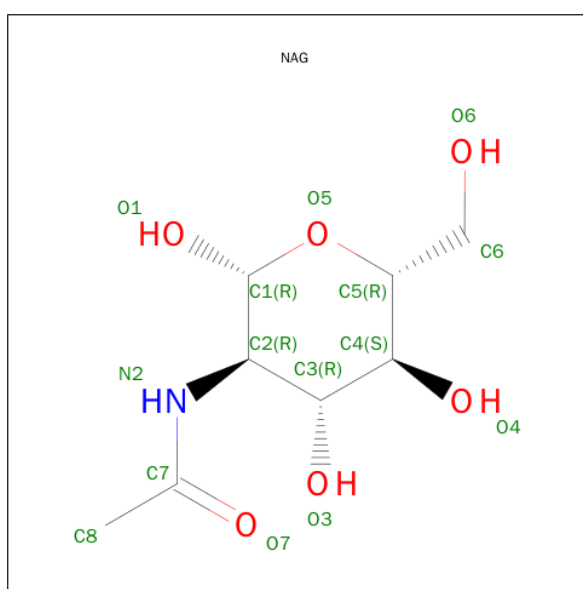
- Molecule 2 is a protein called Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1257	792	210	249	6			
2	D	155	Total	C	N	O	S	0	0	0
			1257	792	210	249	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	SER	CYS	ENGINEERED MUTATION	UNP Q14116
B	68	SER	CYS	ENGINEERED MUTATION	UNP Q14116
B	76	SER	CYS	ENGINEERED MUTATION	UNP Q14116
B	127	SER	CYS	ENGINEERED MUTATION	UNP Q14116
D	38	SER	CYS	ENGINEERED MUTATION	UNP Q14116
D	68	SER	CYS	ENGINEERED MUTATION	UNP Q14116
D	76	SER	CYS	ENGINEERED MUTATION	UNP Q14116
D	127	SER	CYS	ENGINEERED MUTATION	UNP Q14116

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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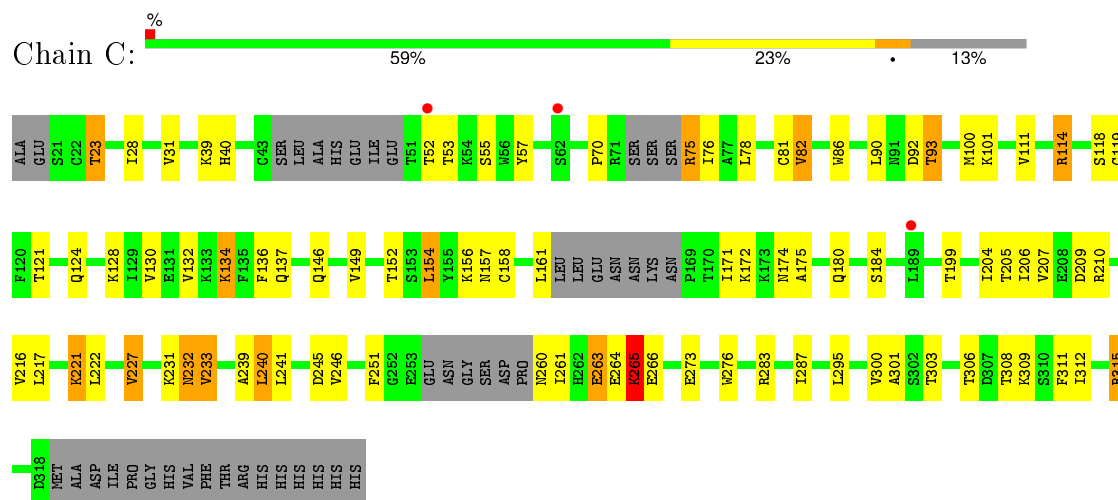
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

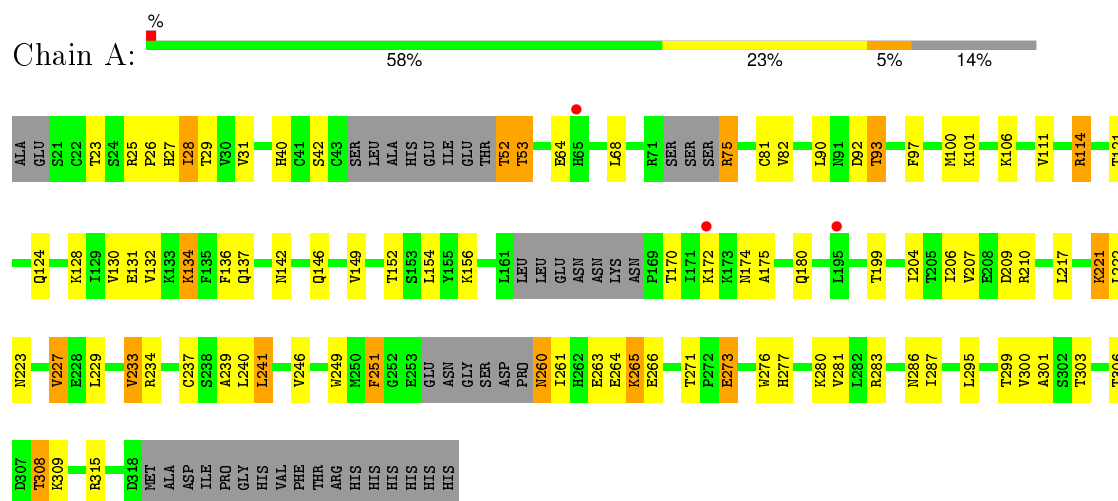
3 Residue-property plots

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.

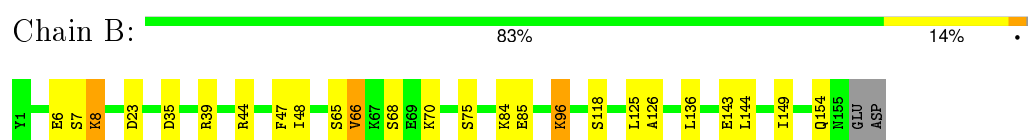
- Molecule 1: Interleukin-18 receptor 1



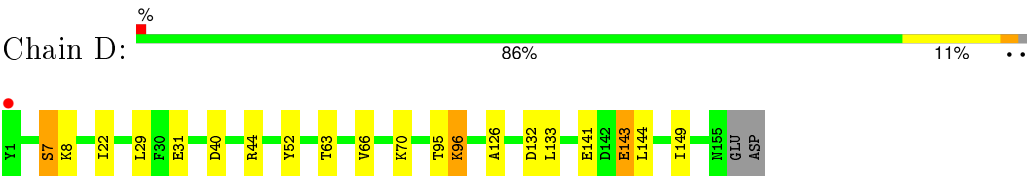
- Molecule 1: Interleukin-18 receptor 1



- Molecule 2: Interleukin-18



● Molecule 2: Interleukin-18



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.39Å 85.60Å 88.12Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	38.90 – 2.80 38.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.90-2.80) 96.1 (38.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.233 , 0.282 0.243 , 0.288	Depositor DCC
R_{free} test set	1289 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31322 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/2282	0.82	1/3078 (0.0%)
1	C	0.61	0/2289	0.82	0/3088
2	B	0.63	0/1278	0.86	4/1713 (0.2%)
2	D	0.61	1/1278 (0.1%)	0.81	2/1713 (0.1%)
All	All	0.62	1/7127 (0.0%)	0.83	7/9592 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	141	GLU	CG-CD	5.12	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	ARG	NE-CZ-NH1	-9.63	115.49	120.30
2	B	44	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	A	265	LYS	N-CA-C	7.78	132.00	111.00
2	D	143	GLU	OE1-CD-OE2	5.65	130.08	123.30
2	D	144	LEU	CB-CG-CD2	-5.53	101.60	111.00
2	B	144	LEU	CA-CB-CG	5.20	127.25	115.30
2	B	6	GLU	OE1-CD-OE2	5.08	129.40	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	264	GLU	Peptide

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	2234	0	2197	47	0
1	C	2241	0	2203	49	0
2	B	1257	0	1249	10	0
2	D	1257	0	1249	7	0
3	A	56	0	52	3	0
3	C	56	0	52	1	0
All	All	7101	0	7002	112	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 8.

All (112) 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:40:HIS:CE1	1:C:81:CYS:HB2	2.06	0.90
1:A:40:HIS:NE2	1:A:81:CYS:HB2	1.87	0.90
1:C:40:HIS:HE1	1:C:81:CYS:HB2	1.33	0.89
1:A:40:HIS:HE2	1:A:81:CYS:HB2	1.37	0.89
1:C:233:VAL:HG22	1:C:287:ILE:HD11	1.60	0.84
1:A:233:VAL:HG22	1:A:287:ILE:HD11	1.62	0.81
1:C:217:LEU:HD23	1:C:239:ALA:HB2	1.76	0.67
1:C:114:ARG:NH1	1:C:114:ARG:HB2	2.12	0.64
2:D:22:ILE:HG23	2:D:44:ARG:HH11	1.62	0.64
1:A:137:GLN:OE1	1:A:172:LYS:NZ	2.31	0.63
1:C:263:GLU:HG3	1:C:283:ARG:CZ	2.30	0.61
1:A:130:VAL:HG11	1:A:136:PHE:HB2	1.83	0.59
1:A:281:VAL:HG21	3:A:403:NAG:H82	1.85	0.59
1:A:295:LEU:O	3:A:404:NAG:H82	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:HB2	1:A:280:LYS:HG3	1.87	0.57
1:A:25:ARG:NH2	1:A:28:ILE:HD12	2.21	0.56
1:C:93:THR:HG22	1:C:111:VAL:HB	1.87	0.56
1:C:146:GLN:O	1:C:149:VAL:HG12	2.06	0.56
2:B:126:ALA:O	2:B:136:LEU:HD12	2.06	0.56
1:C:128:LYS:HB2	1:C:204:ILE:HD13	1.87	0.55
1:C:180:GLN:HE21	1:C:206:ILE:H	1.55	0.55
1:C:132:VAL:O	1:C:175:ALA:HB3	2.07	0.55
1:A:180:GLN:HE21	1:A:206:ILE:H	1.56	0.54
1:C:55:SER:HB3	1:C:57:TYR:CZ	2.42	0.54
1:A:299:THR:OG1	1:A:308:THR:HB	2.08	0.54
1:C:227:VAL:HG11	1:C:233:VAL:HG13	1.89	0.54
1:C:75:ARG:HB3	1:C:86:TRP:O	2.08	0.53
1:A:241:LEU:O	1:A:276:TRP:HB2	2.08	0.53
1:A:251:PHE:CD2	1:A:251:PHE:N	2.77	0.53
1:A:97:PHE:CE1	1:A:106:LYS:HG3	2.44	0.52
2:B:47:PHE:CD1	2:B:66:VAL:HG13	2.44	0.52
1:C:301:ALA:HA	1:C:306:THR:HG22	1.91	0.52
1:A:114:ARG:HB2	1:A:114:ARG:NH1	2.24	0.52
1:A:223:ASN:HD21	1:A:309:LYS:HD3	1.74	0.52
2:B:48:ILE:N	2:B:65:SER:O	2.35	0.52
1:C:130:VAL:HG11	1:C:136:PHE:HB2	1.92	0.52
1:C:137:GLN:OE1	1:C:172:LYS:NZ	2.34	0.51
1:C:265:LYS:HD2	1:C:266:GLU:H	1.76	0.51
2:B:126:ALA:HB2	2:B:149:ILE:HG22	1.92	0.51
1:A:234:ARG:HD3	1:A:283:ARG:HD3	1.92	0.50
1:C:55:SER:HB3	1:C:57:TYR:CE1	2.47	0.50
1:A:261:ILE:HG23	1:A:286:ASN:H	1.77	0.50
1:A:271:THR:OG1	1:A:273:GLU:HG2	2.10	0.50
1:A:40:HIS:CD2	1:A:81:CYS:HB2	2.48	0.49
1:A:227:VAL:HG11	1:A:233:VAL:HG13	1.93	0.49
1:A:132:VAL:O	1:A:175:ALA:HB3	2.13	0.49
1:C:75:ARG:NH2	1:C:92:ASP:OD2	2.45	0.49
1:C:309:LYS:HD2	1:C:311:PHE:CZ	2.47	0.49
1:A:28:ILE:HG13	1:A:29:THR:N	2.28	0.49
1:A:217:LEU:HD23	1:A:239:ALA:HB2	1.96	0.48
1:C:39:LYS:HG3	1:C:82:VAL:HG23	1.96	0.48
2:D:7:SER:O	2:D:8:LYS:HD2	2.14	0.47
1:C:232:ASN:N	1:C:232:ASN:OD1	2.46	0.47
1:A:221:LYS:HD3	1:A:221:LYS:HA	1.72	0.47
2:B:75:SER:CB	2:B:84:LYS:HE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:N	1:A:174:ASN:OD1	2.48	0.47
1:A:93:THR:HG22	1:A:111:VAL:HB	1.97	0.46
1:C:31:VAL:HG13	1:C:114:ARG:HB3	1.98	0.46
1:C:295:LEU:HD22	1:C:312:ILE:HG12	1.98	0.46
1:C:154:LEU:HD23	1:C:184:SER:O	2.15	0.46
1:C:221:LYS:HA	1:C:221:LYS:HD3	1.70	0.46
1:A:146:GLN:O	1:A:149:VAL:HG12	2.16	0.45
1:A:128:LYS:HB2	1:A:204:ILE:HD13	1.98	0.45
1:C:31:VAL:HG23	1:C:124:GLN:HG2	1.98	0.45
1:C:118:SER:OG	1:C:119:CYS:N	2.49	0.45
1:C:70:PRO:HD2	1:C:78:LEU:HD13	1.98	0.45
2:B:96:LYS:HB3	2:B:118:SER:O	2.16	0.45
1:C:114:ARG:CZ	1:C:114:ARG:HB2	2.47	0.45
1:C:295:LEU:O	3:C:804:NAG:O6	2.35	0.44
1:C:128:LYS:HB2	1:C:204:ILE:CD1	2.47	0.44
1:A:223:ASN:ND2	1:A:309:LYS:HD3	2.32	0.44
1:A:237:CYS:HB2	1:A:249:TRP:CZ2	2.52	0.44
1:A:23:THR:OG1	1:A:23:THR:O	2.29	0.44
1:A:75:ARG:NH2	1:A:92:ASP:OD2	2.49	0.44
1:A:52:THR:OG1	1:A:53:THR:N	2.51	0.44
1:A:142:ASN:O	1:A:146:GLN:HB2	2.18	0.43
1:C:157:ASN:O	1:C:158:CYS:HB2	2.18	0.43
1:C:241:LEU:O	1:C:276:TRP:HB2	2.19	0.43
1:C:90:LEU:O	1:C:93:THR:HG23	2.18	0.43
1:C:265:LYS:CD	1:C:266:GLU:H	2.32	0.43
2:B:7:SER:O	2:B:8:LYS:HD2	2.19	0.43
1:A:25:ARG:HA	1:A:26:PRO:HD3	1.86	0.43
2:B:125:LEU:HB3	2:B:136:LEU:HD11	2.02	0.42
1:A:180:GLN:NE2	1:A:206:ILE:H	2.16	0.42
2:D:126:ALA:HB2	2:D:149:ILE:HG22	2.01	0.42
1:A:260:ASN:N	1:A:260:ASN:OD1	2.52	0.42
1:C:114:ARG:HH11	1:C:114:ARG:HB2	1.84	0.42
1:A:264:GLU:HA	1:A:281:VAL:O	2.19	0.42
2:B:75:SER:HB2	2:B:84:LYS:HE2	2.02	0.42
2:D:29:LEU:HD13	2:D:133:LEU:HD22	2.02	0.42
1:A:131:GLU:O	1:A:134:LYS:HB2	2.19	0.42
1:C:23:THR:O	1:C:23:THR:OG1	2.35	0.42
1:A:90:LEU:O	1:A:93:THR:HG23	2.20	0.42
1:C:70:PRO:HG3	1:C:76:ILE:CG2	2.49	0.42
1:C:227:VAL:CG1	1:C:233:VAL:HG13	2.50	0.42
1:A:31:VAL:HG23	1:A:124:GLN:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG23	1:C:124:GLN:CG	2.50	0.41
1:A:180:GLN:CG	1:A:206:ILE:H	2.32	0.41
1:A:277:HIS:HE1	3:A:403:NAG:C6	2.33	0.41
1:C:241:LEU:HB2	1:C:245:ASP:HB2	2.02	0.41
2:D:52:TYR:CE1	2:D:63:THR:HG23	2.55	0.41
1:C:263:GLU:HG3	1:C:283:ARG:NH2	2.35	0.41
1:A:31:VAL:HG13	1:A:114:ARG:HB3	2.02	0.41
1:A:301:ALA:HA	1:A:306:THR:HG22	2.03	0.41
2:B:35:ASP:O	2:B:39:ARG:HB2	2.21	0.41
1:C:171:ILE:HD13	1:C:171:ILE:HA	1.89	0.41
1:A:27:HIS:CE1	2:D:40:ASP:HB3	2.55	0.40
2:D:95:THR:C	2:D:96:LYS:HG3	2.42	0.40
1:C:134:LYS:N	1:C:174:ASN:OD1	2.54	0.40
1:C:261:ILE:O	1:C:261:ILE:HG22	2.20	0.40
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.85	0.40
1:C:240:LEU:HD12	1:C:240:LEU:HA	1.85	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	264/317 (83%)	240 (91%)	22 (8%)	2 (1%)	24	58
1	C	265/317 (84%)	240 (91%)	23 (9%)	2 (1%)	24	58
2	B	153/157 (98%)	146 (95%)	7 (5%)	0	100	100
2	D	153/157 (98%)	147 (96%)	5 (3%)	1 (1%)	26	62
All	All	835/948 (88%)	773 (93%)	57 (7%)	5 (1%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	143	GLU
1	A	265	LYS
1	A	64	GLU
1	C	265	LYS
1	C	315	ARG

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	255/293 (87%)	218 (86%)	37 (14%)	4	11
1	C	256/293 (87%)	218 (85%)	38 (15%)	4	11
2	B	146/148 (99%)	137 (94%)	9 (6%)	23	54
2	D	146/148 (99%)	140 (96%)	6 (4%)	37	72
All	All	803/882 (91%)	713 (89%)	90 (11%)	7	22

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	THR
1	C	28	ILE
1	C	52	THR
1	C	53	THR
1	C	75	ARG
1	C	82	VAL
1	C	93	THR
1	C	100	MET
1	C	101	LYS
1	C	114	ARG
1	C	121	THR
1	C	134	LYS
1	C	152	THR
1	C	154	LEU
1	C	156	LYS
1	C	199	THR
1	C	205	THR

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Mol	Chain	Res	Type
1	C	207	VAL
1	C	209	ASP
1	C	210	ARG
1	C	216	VAL
1	C	221	LYS
1	C	222	LEU
1	C	227	VAL
1	C	231	LYS
1	C	232	ASN
1	C	233	VAL
1	C	240	LEU
1	C	246	VAL
1	C	251	PHE
1	C	260	ASN
1	C	263	GLU
1	C	265	LYS
1	C	273	GLU
1	C	300	VAL
1	C	303	THR
1	C	308	THR
1	C	315	ARG
1	A	28	ILE
1	A	42	SER
1	A	52	THR
1	A	53	THR
1	A	68	LEU
1	A	75	ARG
1	A	82	VAL
1	A	93	THR
1	A	100	MET
1	A	101	LYS
1	A	114	ARG
1	A	121	THR
1	A	134	LYS
1	A	152	THR
1	A	154	LEU
1	A	156	LYS
1	A	170	THR
1	A	199	THR
1	A	207	VAL
1	A	209	ASP
1	A	210	ARG

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Mol	Chain	Res	Type
1	A	221	LYS
1	A	222	LEU
1	A	227	VAL
1	A	229	LEU
1	A	233	VAL
1	A	240	LEU
1	A	241	LEU
1	A	246	VAL
1	A	251	PHE
1	A	260	ASN
1	A	263	GLU
1	A	273	GLU
1	A	300	VAL
1	A	303	THR
1	A	308	THR
1	A	315	ARG
2	B	8	LYS
2	B	23	ASP
2	B	66	VAL
2	B	68	SER
2	B	70	LYS
2	B	85	GLU
2	B	96	LYS
2	B	143	GLU
2	B	154	GLN
2	D	7	SER
2	D	31	GLU
2	D	66	VAL
2	D	70	LYS
2	D	96	LYS
2	D	132	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	40	HIS
1	C	180	GLN
1	A	180	GLN
2	B	26	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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$
3	NAG	A	401	1	14,14,15	0.94	1 (7%)	15,19,21	0.79	1 (6%)
3	NAG	A	402	1	14,14,15	1.52	1 (7%)	15,19,21	0.85	1 (6%)
3	NAG	A	403	1	14,14,15	0.35	0	15,19,21	1.02	0
3	NAG	A	404	1	14,14,15	1.10	1 (7%)	15,19,21	1.13	1 (6%)
3	NAG	C	801	1	14,14,15	1.72	3 (21%)	15,19,21	0.92	1 (6%)
3	NAG	C	802	1	14,14,15	0.94	2 (14%)	15,19,21	0.80	1 (6%)
3	NAG	C	803	1	14,14,15	0.91	1 (7%)	15,19,21	0.66	0
3	NAG	C	804	1	14,14,15	1.16	1 (7%)	15,19,21	1.19	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
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1	-	0/6/23/26	0/1/1/1
3	NAG	A	404	1	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1	-	0/6/23/26	0/1/1/1
3	NAG	C	804	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	NAG	O5-C1	-3.98	1.37	1.43
3	C	802	NAG	O5-C1	2.17	1.47	1.43
3	C	802	NAG	C1-C2	2.18	1.55	1.52
3	A	401	NAG	C1-C2	2.70	1.56	1.52
3	C	801	NAG	C1-C2	2.92	1.56	1.52
3	C	803	NAG	C1-C2	2.95	1.56	1.52
3	A	404	NAG	O5-C1	3.59	1.49	1.43
3	C	801	NAG	C2-N2	3.68	1.52	1.46
3	C	804	NAG	C1-C2	4.17	1.58	1.52
3	A	402	NAG	O5-C1	5.34	1.52	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	NAG	C1-O5-C5	-2.99	108.46	112.25
3	A	401	NAG	O3-C3-C2	-2.43	104.30	109.11
3	A	402	NAG	C1-O5-C5	2.43	115.34	112.25
3	C	802	NAG	C1-O5-C5	2.44	115.34	112.25
3	C	804	NAG	O3-C3-C2	3.47	115.98	109.11
3	A	404	NAG	C1-O5-C5	3.75	117.01	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	NAG	2	0
3	A	404	NAG	1	0
3	C	804	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	274/317 (86%)	0.02	3 (1%) 82 74	46, 61, 95, 118	0
1	C	275/317 (86%)	0.06	3 (1%) 82 74	44, 62, 91, 129	0
2	B	155/157 (98%)	-0.23	0 100 100	29, 45, 81, 92	0
2	D	155/157 (98%)	-0.23	1 (0%) 90 86	32, 48, 85, 118	0
All	All	859/948 (90%)	-0.06	7 (0%) 87 81	29, 57, 91, 129	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	SER	4.0
1	A	172	LYS	3.3
1	C	52	THR	3.1
1	A	65	HIS	3.0
1	C	189	LEU	2.4
1	A	195	LEU	2.3
2	D	1	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	803	14/15	0.90	0.28	4.02	54,54,54,54	0
3	NAG	A	402	14/15	0.76	0.28	3.64	54,54,54,54	0
3	NAG	A	403	14/15	0.82	0.26	3.49	54,54,54,54	0
3	NAG	C	802	14/15	0.88	0.19	0.75	54,54,54,54	0
3	NAG	C	801	14/15	0.81	0.24	0.51	54,54,54,54	0
3	NAG	C	804	14/15	0.78	0.20	0.15	54,54,54,54	0
3	NAG	A	401	14/15	0.86	0.22	-0.14	54,54,54,54	0
3	NAG	A	404	14/15	0.83	0.14	-1.04	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.