Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:16 AM GMT

PDB ID	:	3O95
Title	:	Crystal Structure of Human DPP4 Bound to TAK-100
Authors	:	Yano, J.K.; Aertgeerts, K.
Deposited on	:	2010-08-03
Resolution	:	2.85 Å(reported)

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

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

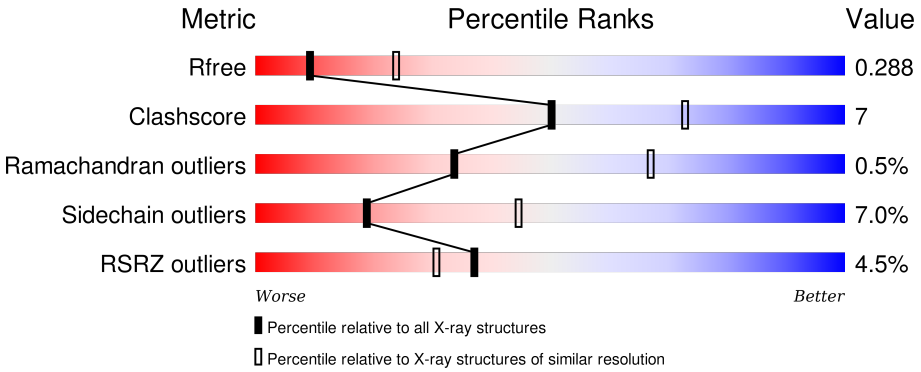
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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 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	740	4% 77% 19%
1	B	740	% 78% 19%
1	C	740	8% 78% 19%
1	D	740	4% 76% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	901	X	-	-	-
3	NAG	B	3211	-	-	-	X
3	NAG	D	5201	X	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24870 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

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

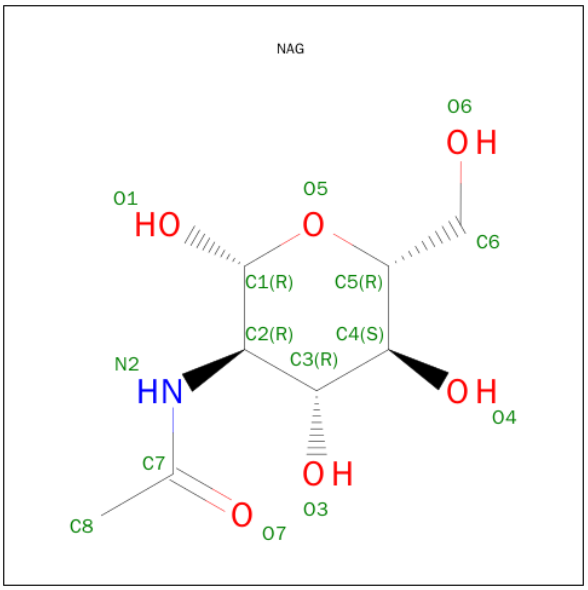
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

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

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



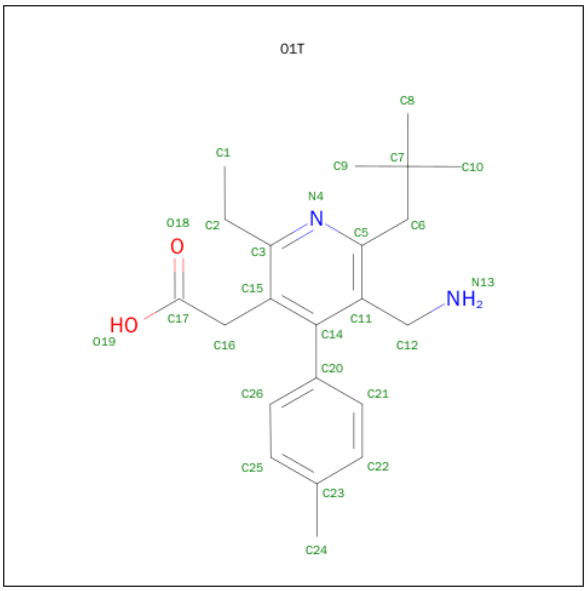
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	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 [5-(AMINOMETHYL)-6-(2,2-DIMETHYLPROPYL)-2-ETHYL-4-(4-METHYLPHENYL)PYRIDIN-3-YL]ACETIC ACID (three-letter code: 01T) (formula: $C_{22}H_{30}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 26 22 2 2	0	0
4	B	1	Total C N O 26 22 2 2	0	0
4	C	1	Total C N O 26 22 2 2	0	0
4	D	1	Total C N O 26 22 2 2	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	3	Total C N O 42 24 3 15	0	0

- Molecule 6 is water.

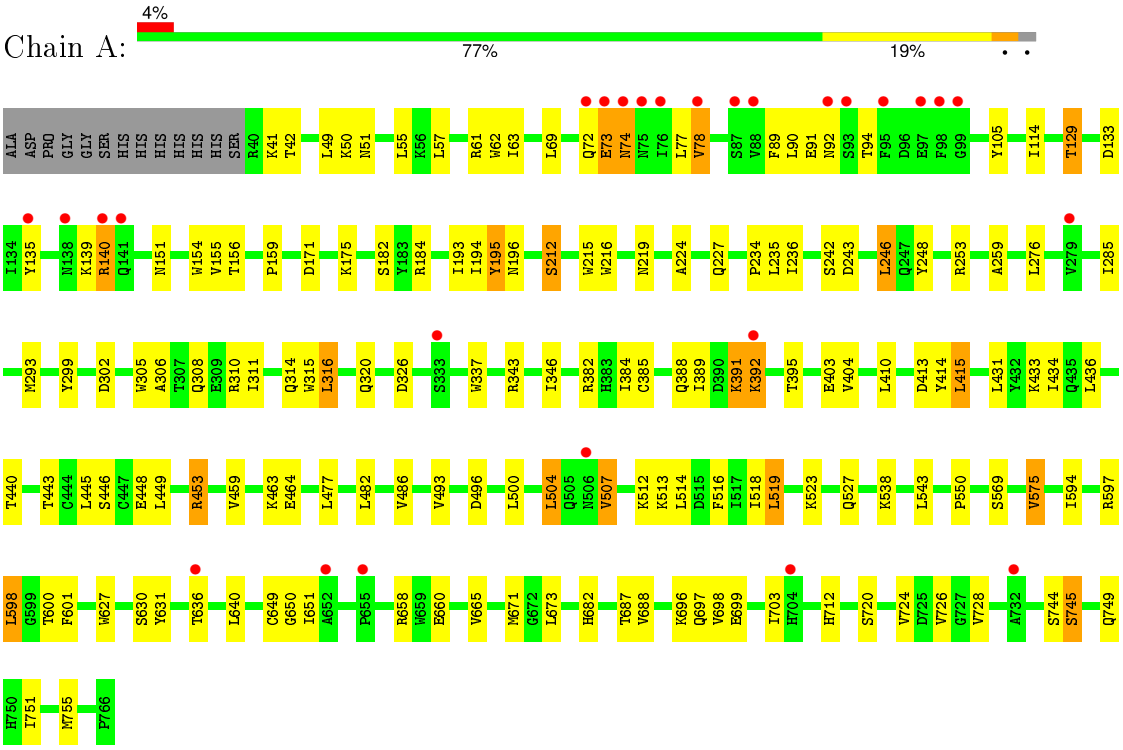
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	145	Total O 145 145	0	0
6	B	134	Total O 134 134	0	0
6	C	76	Total O 76 76	0	0
6	D	132	Total O 132 132	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

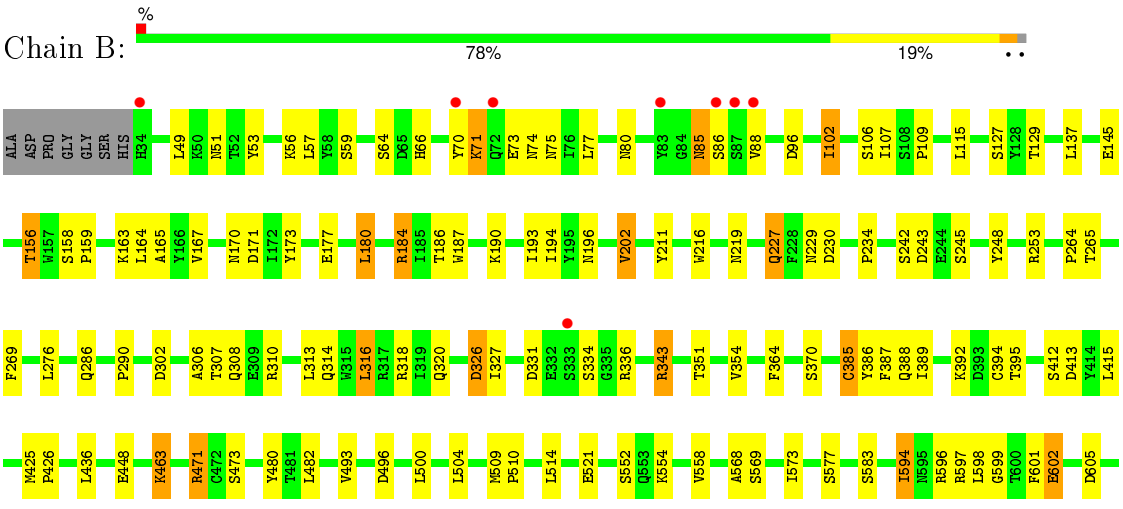
- Molecule 1: Dipeptidyl peptidase 4

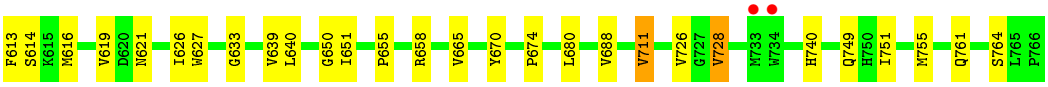
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

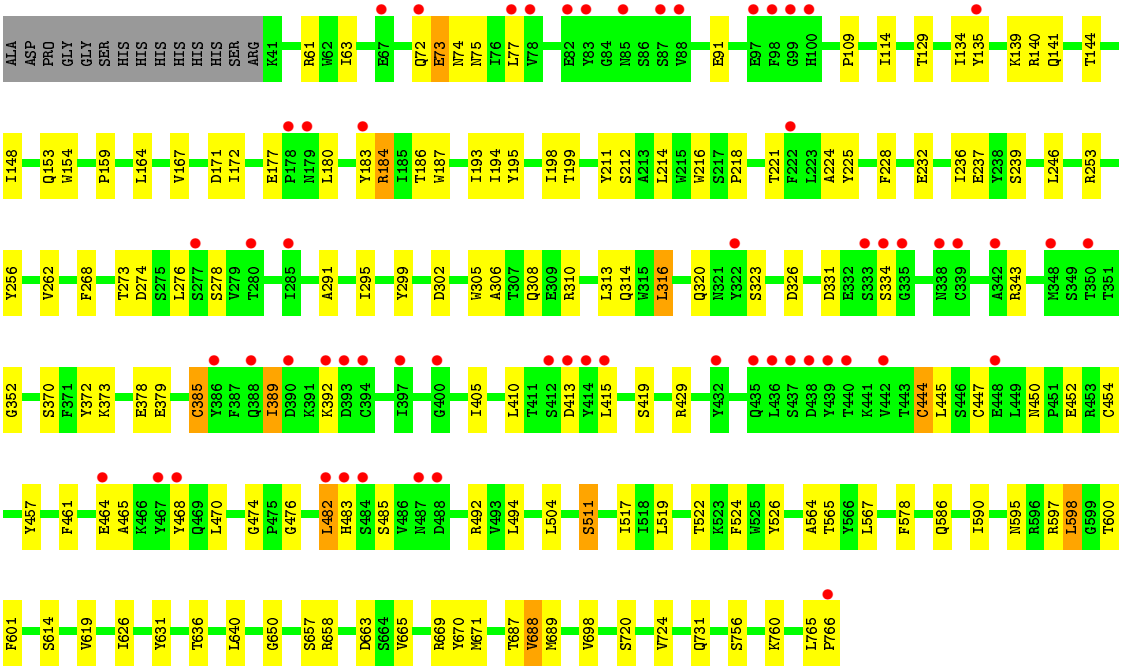
Chain B:





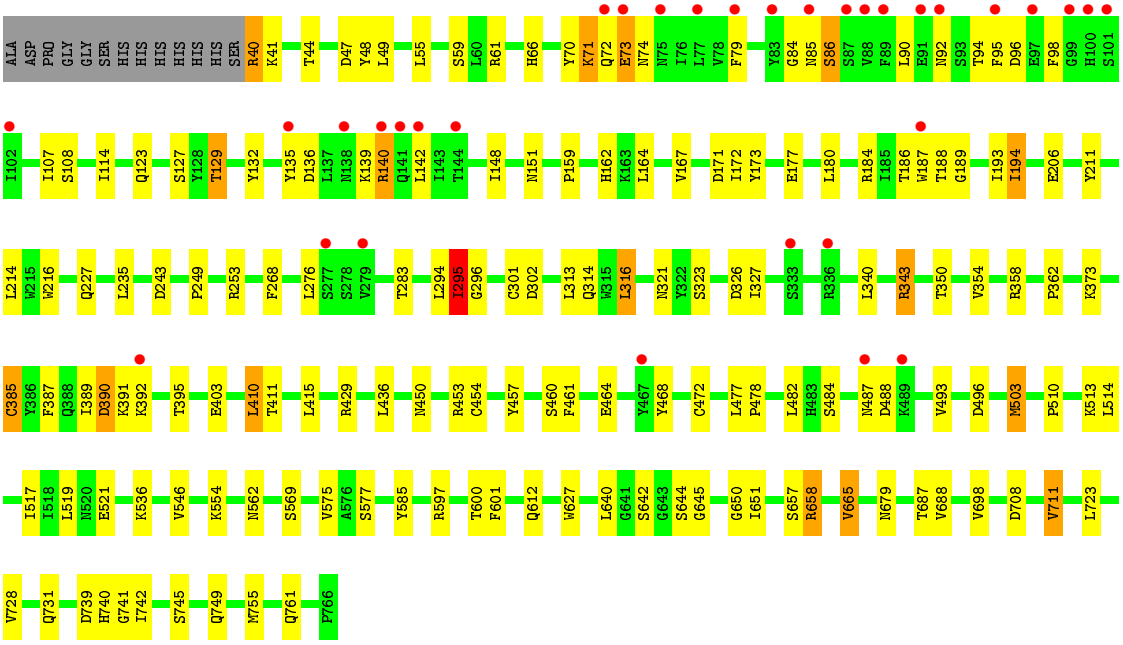
• Molecule 1: Dipeptidyl peptidase 4

Chain C:



• Molecule 1: Dipeptidyl peptidase 4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.72Å 123.33Å 144.42Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	35.00 – 2.85 34.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.00-2.85) 99.2 (34.83-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.248 0.242 , 0.288	Depositor DCC
R_{free} test set	4489 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.8	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 89524 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24870	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 01T, 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	0.55	1/6129 (0.0%)	0.62	0/8336
1	B	0.52	0/6190	0.61	0/8419
1	C	0.49	0/6118	0.59	0/8322
1	D	0.54	0/6129	0.61	0/8336
All	All	0.52	1/24566 (0.0%)	0.61	0/33413

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
2	B	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	GLN	CD-OE1	5.07	1.35	1.24

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	901	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5957	0	5673	87	0
1	B	6013	0	5714	81	0
1	C	5946	0	5663	81	0
1	D	5957	0	5674	87	0
2	A	112	0	100	0	0
2	B	56	0	50	2	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
3	C	42	0	39	0	0
3	D	56	0	52	1	0
4	A	26	0	29	2	0
4	B	26	0	29	1	0
4	C	26	0	29	0	0
4	D	26	0	29	1	0
5	C	42	0	37	1	0
6	A	145	0	0	1	0
6	B	134	0	0	3	0
6	C	76	0	0	2	0
6	D	132	0	0	6	0
All	All	24870	0	23208	332	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 7.

All (332) 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:193:ILE:HG22	1:D:194:ILE:HD13	1.49	0.94
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.94	0.91
3:D:2811:NAG:H2	6:D:845:HOH:O	1.70	0.89
1:C:511:SER:HB3	6:C:812:HOH:O	1.74	0.88
1:B:73:GLU:HA	6:B:866:HOH:O	1.79	0.82
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.64	0.81
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.66	0.78
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.78	0.77
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.20	0.76
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.78	0.76
1:A:91:GLU:O	1:A:94:THR:HG22	1.86	0.75
1:C:72:GLN:O	1:C:73:GLU:HB2	1.86	0.75
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.33	0.73
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.89	0.71
1:B:77:LEU:HD23	1:B:86:SER:HB2	1.72	0.71
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.71	0.71
1:B:614:SER:HA	1:B:619:VAL:HB	1.73	0.70
1:A:343:ARG:HD3	1:A:389:ILE:CG2	2.21	0.69
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.74	0.69
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.74	0.69
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.76	0.68
1:A:343:ARG:HD3	1:A:389:ILE:HG23	1.75	0.67
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.77	0.66
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.78	0.66
1:C:184:ARG:HD3	1:C:186:THR:O	1.96	0.66
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.78	0.65
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.77	0.65
1:B:290:PRO:HG3	1:B:326:ASP:OD1	1.97	0.64
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.28	0.64
2:B:901:NAG:H61	2:B:902:NAG:C7	2.29	0.63
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.62	0.63
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.34	0.62
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.80	0.62
1:B:471:ARG:HG2	1:B:480:TYR:CE1	2.34	0.62
1:A:74:ASN:HB2	1:A:92:ASN:HB3	1.80	0.62
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.35	0.62
1:D:84:GLY:C	1:D:86:SER:H	2.03	0.62
1:A:751:ILE:O	1:A:755:MET:HG3	2.00	0.61
1:D:723:LEU:HD22	1:D:728:VAL:HG11	1.82	0.61
1:B:316:LEU:HD13	1:B:320:GLN:HG2	1.83	0.60
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.37	0.60
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.82	0.60
1:B:184:ARG:HD3	1:B:186:THR:O	2.01	0.59
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.36	0.59
1:C:614:SER:HA	1:C:619:VAL:HB	1.83	0.59
1:C:177:GLU:HB2	1:C:180:LEU:HG	1.83	0.59
1:D:723:LEU:HB3	1:D:728:VAL:HG13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:SER:OG	1:B:243:ASP:N	2.36	0.59
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.38	0.58
1:B:613:PHE:O	1:B:616:MET:HB2	2.03	0.58
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.85	0.58
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.03	0.58
1:C:167:VAL:HA	1:C:171:ASP:O	2.03	0.58
1:B:73:GLU:O	1:B:74:ASN:HB2	2.04	0.57
1:D:70:TYR:CE2	1:D:71:LYS:HE3	2.40	0.57
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.39	0.57
1:C:72:GLN:O	1:C:73:GLU:CB	2.53	0.57
1:A:72:GLN:O	1:A:73:GLU:HB2	2.05	0.57
1:D:72:GLN:C	1:D:74:ASN:H	2.08	0.56
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.88	0.56
1:C:657:SER:HA	1:C:688:VAL:CG1	2.36	0.56
1:D:206:GLU:HB3	1:D:665:VAL:CG2	2.35	0.56
1:C:172:ILE:HD13	1:C:214:LEU:HD21	1.88	0.56
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.88	0.56
1:B:127:SER:HB3	1:B:211:TYR:CG	2.41	0.55
1:B:202:VAL:HG22	6:B:799:HOH:O	2.05	0.55
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.36	0.55
1:B:554:LYS:HE3	6:B:797:HOH:O	2.06	0.55
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.88	0.55
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.37	0.55
1:A:253:ARG:NH2	1:B:253:ARG:HH21	2.04	0.55
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.41	0.55
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.90	0.54
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.08	0.53
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.90	0.53
1:B:751:ILE:O	1:B:755:MET:HG3	2.07	0.53
1:A:518:ILE:O	1:A:519:LEU:HD13	2.08	0.53
1:A:433:LYS:HD2	1:A:445:LEU:HD21	1.90	0.53
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.90	0.53
1:C:598:LEU:HG	1:C:631:TYR:OH	2.07	0.53
1:B:64:SER:O	1:B:463:LYS:HB2	2.09	0.53
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.90	0.53
1:D:73:GLU:O	1:D:74:ASN:HB2	2.09	0.53
1:B:493:VAL:HG11	1:B:496:ASP:HB3	1.91	0.53
1:A:63:ILE:HD11	1:A:69:LEU:HG	1.92	0.52
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.90	0.52
1:A:242:SER:OG	1:A:243:ASP:N	2.41	0.52
1:C:465:ALA:O	1:C:485:SER:OG	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:GLN:HB3	6:D:880:HOH:O	2.10	0.52
1:B:626:ILE:HD13	1:B:639:VAL:HG11	1.91	0.52
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.74	0.52
1:A:129:THR:HG23	1:A:151:ASN:HA	1.91	0.52
1:B:102:ILE:HD12	1:B:102:ILE:H	1.75	0.51
1:D:184:ARG:HD3	1:D:186:THR:O	2.10	0.51
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.92	0.51
1:A:598:LEU:HG	1:A:631:TYR:OH	2.11	0.51
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.44	0.51
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.45	0.51
1:D:79:PHE:HA	1:D:86:SER:HB3	1.93	0.51
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.93	0.51
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.93	0.51
1:A:550:PRO:HB3	1:A:594:ILE:HD11	1.92	0.51
1:C:731:GLN:NE2	1:D:731:GLN:OE1	2.44	0.51
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.40	0.50
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.46	0.50
1:C:75:ASN:HD22	1:C:91:GLU:HG2	1.76	0.50
1:D:410:LEU:HD22	1:D:411:THR:O	2.11	0.50
1:A:346:ILE:H	1:A:392:LYS:NZ	2.09	0.50
1:B:471:ARG:CG	1:B:480:TYR:CE1	2.94	0.50
1:C:522:THR:HB	1:C:524:PHE:CE2	2.46	0.50
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.46	0.50
1:D:389:ILE:HG22	1:D:390:ASP:OD1	2.12	0.50
1:D:107:ILE:HG22	1:D:108:SER:O	2.11	0.50
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.92	0.50
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.47	0.50
1:D:189:GLY:HA2	1:D:194:ILE:HG22	1.94	0.50
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.45	0.49
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.42	0.49
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.42	0.49
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.94	0.49
1:C:756:SER:O	1:C:760:LYS:HG3	2.12	0.49
1:A:42:THR:HB	1:A:569:SER:OG	2.12	0.49
1:A:63:ILE:CD1	1:A:69:LEU:HG	2.42	0.49
1:C:586:GLN:HB3	1:C:590:ILE:HD12	1.95	0.49
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.49
1:A:154:TRP:CD1	1:A:212:SER:HB2	2.47	0.49
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.95	0.49
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.93	0.49
1:B:651:ILE:HD13	1:B:755:MET:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ARG:HD3	1:C:389:ILE:HG23	1.94	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.48
1:C:195:TYR:CD1	1:C:195:TYR:N	2.81	0.48
1:C:91:GLU:HB3	6:C:818:HOH:O	2.12	0.48
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.94	0.48
1:C:482:LEU:HB2	1:C:494:LEU:HD21	1.94	0.48
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.28	0.48
1:D:127:SER:HB3	1:D:211:TYR:CG	2.48	0.48
1:B:331:ASP:HB3	1:B:334:SER:HB2	1.95	0.48
1:B:243:ASP:OD2	1:B:245:SER:HB2	2.13	0.48
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.29	0.48
1:D:268:PHE:CD2	1:D:313:LEU:HD11	2.48	0.48
1:C:221:THR:HG23	1:C:274:ASP:OD2	2.12	0.48
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.95	0.48
1:B:334:SER:HB3	1:B:336:ARG:H	1.78	0.47
1:C:291:ALA:O	1:C:295:ILE:HG23	2.14	0.47
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.50	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.47
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.95	0.47
1:C:139:LYS:HB2	1:C:141:GLN:HG2	1.96	0.47
1:B:674:PRO:O	1:B:680:LEU:HD13	2.15	0.47
1:C:268:PHE:CE2	1:C:313:LEU:HD11	2.48	0.47
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.95	0.47
1:C:372:TYR:HA	1:C:385:CYS:O	2.15	0.47
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.15	0.47
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.14	0.47
1:A:744:SER:O	1:A:745:SER:C	2.54	0.47
1:A:195:TYR:N	1:A:195:TYR:CD1	2.82	0.47
1:D:642:SER:OG	1:D:644:SER:HB3	2.15	0.47
1:A:299:TYR:CE1	1:A:665:VAL:HG22	2.50	0.46
1:B:568:ALA:HA	1:B:573:ILE:O	2.15	0.46
1:B:170:ASN:O	1:B:196:ASN:HB2	2.15	0.46
1:C:195:TYR:HB3	1:C:198:ILE:HG13	1.97	0.46
1:D:600:THR:OG1	1:D:601:PHE:N	2.47	0.46
1:D:294:LEU:C	1:D:296:GLY:H	2.19	0.46
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.97	0.46
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.98	0.46
1:B:599:GLY:N	1:B:602:GLU:OE2	2.37	0.46
1:B:415:LEU:HD23	1:B:415:LEU:C	2.35	0.46
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.98	0.46
1:D:708:ASP:OD1	1:D:740:HIS:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:HD2	1:B:389:ILE:HG23	1.97	0.46
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.97	0.46
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.97	0.46
1:D:194:ILE:HG13	2:D:2291:NAG:H82	1.98	0.46
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.15	0.46
1:C:429:ARG:HB2	1:C:457:TYR:H	1.81	0.46
1:C:444:CYS:SG	1:C:445:LEU:N	2.88	0.46
1:D:44:THR:O	1:D:47:ASP:HB2	2.15	0.46
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.51	0.45
1:B:109:PRO:HG2	1:B:158:SER:O	2.16	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.47	0.45
1:C:405:ILE:HG12	1:C:419:SER:HA	1.97	0.45
1:D:450:ASN:O	1:D:454:CYS:HB2	2.16	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:C:218:PRO:HD3	1:C:305:TRP:HB3	1.98	0.45
1:A:253:ARG:HH21	1:B:253:ARG:NH2	2.08	0.45
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.99	0.45
1:D:301:CYS:SG	1:D:316:LEU:HB2	2.57	0.45
1:D:139:LYS:O	1:D:139:LYS:HG2	2.15	0.45
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.97	0.45
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.98	0.45
1:D:132:TYR:HB2	1:D:148:ILE:HG21	1.98	0.45
1:D:162:HIS:NE2	1:D:177:GLU:OE2	2.45	0.45
1:C:464:GLU:O	1:C:464:GLU:HG3	2.16	0.45
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.99	0.45
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.30	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.17	0.45
1:A:171:ASP:OD1	1:A:184:ARG:NH2	2.50	0.45
1:B:71:LYS:HA	1:B:75:ASN:O	2.17	0.45
1:A:139:LYS:O	1:A:140:ARG:HB2	2.17	0.45
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.47	0.45
1:B:156:THR:HG23	1:B:165:ALA:HB3	1.99	0.45
1:D:640:LEU:HB3	1:D:698:VAL:HG21	1.99	0.44
1:A:433:LYS:HB3	1:A:445:LEU:HD11	1.99	0.44
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.52	0.44
1:D:136:ASP:CG	1:D:139:LYS:HB3	2.37	0.44
1:B:425:MET:HA	1:B:426:PRO:HD3	1.80	0.44
1:B:473:SER:HB3	1:B:558:VAL:HG13	1.99	0.44
1:D:484:SER:O	1:D:488:ASP:HA	2.17	0.44
1:A:453:ARG:NH2	1:A:477:LEU:O	2.41	0.44
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:HD13	1:C:320:GLN:HG2	1.99	0.44
1:C:352:GLY:HA2	1:C:595:ASN:OD1	2.17	0.44
1:A:293:MET:HG3	1:A:315:TRP:HB2	1.98	0.44
6:A:859:HOH:O	1:D:40:ARG:HG2	2.17	0.44
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.52	0.44
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.98	0.44
1:D:321:ASN:ND2	6:D:843:HOH:O	2.49	0.44
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.48	0.44
1:C:199:THR:HA	1:C:228:PHE:CE2	2.53	0.44
1:C:474:GLY:HA2	1:C:476:GLY:O	2.18	0.44
1:D:167:VAL:HA	1:D:171:ASP:O	2.18	0.44
1:D:173:TYR:CE1	1:D:184:ARG:HG3	2.53	0.43
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.99	0.43
1:C:232:GLU:HB2	1:C:262:VAL:HG11	2.00	0.43
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.43
1:A:703:ILE:HG21	1:A:751:ILE:HD12	2.00	0.43
1:C:657:SER:HA	1:C:688:VAL:HG12	1.99	0.43
1:C:218:PRO:HD3	1:C:305:TRP:CB	2.49	0.43
1:D:487:ASN:O	1:D:488:ASP:HB2	2.17	0.43
1:C:236:ILE:HD12	1:D:249:PRO:HD2	2.00	0.43
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.99	0.43
1:D:645:GLY:HA2	6:D:841:HOH:O	2.18	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HB3	2.01	0.43
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.01	0.43
1:B:53:TYR:HB3	1:B:500:LEU:CD1	2.48	0.43
1:A:215:TRP:HB2	1:A:224:ALA:HB3	1.99	0.43
1:B:307:THR:OG1	1:B:310:ARG:HB3	2.18	0.43
1:B:219:ASN:HB3	1:B:308:GLN:NE2	2.33	0.43
1:D:385:CYS:HB3	1:D:387:PHE:CE2	2.53	0.43
1:A:636:THR:HG21	1:A:651:ILE:O	2.18	0.43
1:C:720:SER:O	1:C:724:VAL:HG23	2.19	0.43
1:D:657:SER:HA	1:D:688:VAL:HG13	1.99	0.43
1:D:453:ARG:HD2	1:D:477:LEU:O	2.19	0.43
1:A:446:SER:HA	1:A:449:LEU:HG	2.01	0.43
1:B:167:VAL:HA	1:B:171:ASP:O	2.19	0.43
1:B:318:ARG:O	1:B:320:GLN:HG3	2.19	0.43
1:C:153:GLN:HB3	1:C:211:TYR:CE1	2.54	0.43
1:B:59:SER:O	1:B:70:TYR:CD1	2.72	0.43
1:A:431:LEU:HD13	1:A:459:VAL:HG11	2.01	0.42
1:A:62:TRP:C	1:A:63:ILE:HD12	2.40	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.49	0.42
1:D:554:LYS:HB3	1:D:577:SER:HB3	2.02	0.42
1:A:391:LYS:HE2	1:A:391:LYS:HB3	1.85	0.42
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.84	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.55	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.42
1:C:183:TYR:CD2	1:C:276:LEU:HD23	2.55	0.42
1:C:598:LEU:HD22	1:C:671:MET:HG2	2.01	0.42
1:A:598:LEU:HD22	1:A:671:MET:HG2	2.01	0.42
1:A:219:ASN:HB3	1:A:308:GLN:HE22	1.85	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.42
1:D:562:ASN:HB2	6:D:869:HOH:O	2.20	0.42
1:D:142:LEU:H	1:D:142:LEU:HD23	1.84	0.42
1:C:564:ALA:HA	1:C:567:LEU:HD12	2.02	0.42
1:A:316:LEU:HD13	1:A:320:GLN:HG2	2.02	0.42
1:B:177:GLU:HB2	1:B:180:LEU:HD22	2.02	0.42
1:A:543:LEU:O	1:A:575:VAL:HA	2.19	0.42
1:C:657:SER:HB2	1:C:689:MET:SD	2.60	0.42
1:A:219:ASN:HB3	1:A:308:GLN:NE2	2.35	0.42
1:C:194:ILE:HD13	5:C:2291:NAG:H82	2.01	0.42
4:D:1:01T:C26	4:D:1:01T:H12	2.49	0.42
1:A:597:ARG:HH11	1:A:682:HIS:CB	2.32	0.41
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.41
1:A:49:LEU:HD22	1:A:749:GLN:HA	2.01	0.41
1:A:382:ARG:H	1:A:403:GLU:HG2	1.85	0.41
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.02	0.41
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.55	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.86	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:A:90:LEU:CD2	1:A:114:ILE:HD13	2.50	0.41
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.41
1:C:114:ILE:HG22	1:C:135:TYR:HB2	2.02	0.41
1:B:552:SER:O	1:B:583:SER:HB2	2.20	0.41
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.55	0.41
1:D:651:ILE:HD13	1:D:755:MET:HG2	2.02	0.41
1:D:739:ASP:HB2	6:D:828:HOH:O	2.21	0.41
1:C:73:GLU:HB3	1:C:74:ASN:H	1.65	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.41
1:D:314:GLN:OE1	1:D:362:PRO:HD3	2.19	0.41
1:A:720:SER:O	1:A:724:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:MET:HG2	1:D:503:MET:H	1.46	0.41
1:A:600:THR:OG1	1:A:601:PHE:N	2.51	0.41
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.56	0.41
1:A:285:ILE:HG21	1:A:337:TRP:HD1	1.86	0.41
1:B:633:GLY:HA3	1:B:655:PRO:HB3	2.03	0.41
1:A:493:VAL:HG11	1:A:496:ASP:HB3	2.03	0.41
1:D:295:ILE:O	1:D:295:ILE:HG23	2.21	0.41
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.56	0.41
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.02	0.41
4:B:1:01T:H12A	4:B:1:01T:H6A	1.90	0.41
1:D:139:LYS:O	1:D:140:ARG:HB2	2.20	0.41
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.02	0.41
1:A:630:SER:OG	4:A:1:01T:C22	2.69	0.41
1:B:601:PHE:O	1:B:605:ASP:N	2.47	0.41
1:B:386:TYR:O	1:B:394:CYS:HB2	2.21	0.41
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.56	0.41
1:B:80:ASN:HB2	1:B:85:ASN:HB2	2.03	0.41
1:A:414:TYR:CD2	1:A:433:LYS:HE2	2.56	0.41
1:B:102:ILE:H	1:B:102:ILE:CD1	2.34	0.41
4:A:1:01T:H6A	4:A:1:01T:H12A	1.84	0.41
1:C:154:TRP:CD2	1:C:212:SER:HB3	2.56	0.41
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.02	0.41
1:D:493:VAL:HG11	1:D:496:ASP:HB3	2.02	0.40
1:D:429:ARG:HB2	1:D:457:TYR:H	1.86	0.40
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.21	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.02	0.40
1:C:517:ILE:HD11	1:C:578:PHE:CE1	2.56	0.40
1:C:626:ILE:HG12	1:C:636:THR:HG23	2.03	0.40
1:B:49:LEU:HB3	1:B:749:GLN:HG2	2.03	0.40
1:D:129:THR:HG23	1:D:151:ASN:HA	2.04	0.40
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.56	0.40
1:B:594:ILE:HG12	1:B:598:LEU:HD23	2.03	0.40
1:C:658:ARG:CB	1:C:687:THR:HG22	2.50	0.40
1:C:299:TYR:CE1	1:C:665:VAL:HG22	2.56	0.40
1:D:741:GLY:O	1:D:742:ILE:C	2.59	0.40
2:B:2291:NAG:H62	2:B:2292:NAG:N2	2.36	0.40
1:C:450:ASN:O	1:C:454:CYS:HB2	2.22	0.40
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.03	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	725/740 (98%)	674 (93%)	47 (6%)	4 (1%)	30	63
1	B	731/740 (99%)	682 (93%)	47 (6%)	2 (0%)	46	76
1	C	724/740 (98%)	667 (92%)	54 (8%)	3 (0%)	39	71
1	D	725/740 (98%)	675 (93%)	44 (6%)	6 (1%)	24	56
All	All	2905/2960 (98%)	2698 (93%)	192 (7%)	15 (0%)	34	67

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	85	ASN
1	C	73	GLU
1	D	85	ASN
1	D	140	ARG
1	A	140	ARG
1	D	73	GLU
1	D	86	SER
1	D	521	GLU
1	A	745	SER
1	B	88	VAL
1	C	389	ILE
1	C	109	PRO
1	A	486	VAL
1	D	295	ILE

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	652/662 (98%)	607 (93%)	45 (7%)	19 45
1	B	658/662 (99%)	608 (92%)	50 (8%)	16 40
1	C	651/662 (98%)	617 (95%)	34 (5%)	29 60
1	D	652/662 (98%)	598 (92%)	54 (8%)	14 36
All	All	2613/2648 (99%)	2430 (93%)	183 (7%)	19 44

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	50	LYS
1	A	51	ASN
1	A	57	LEU
1	A	61	ARG
1	A	74	ASN
1	A	77	LEU
1	A	78	VAL
1	A	129	THR
1	A	133	ASP
1	A	155	VAL
1	A	156	THR
1	A	195	TYR
1	A	212	SER
1	A	235	LEU
1	A	246	LEU
1	A	276	LEU
1	A	316	LEU
1	A	326	ASP
1	A	385	CYS
1	A	388	GLN
1	A	391	LYS
1	A	392	LYS
1	A	395	THR
1	A	410	LEU
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	443	THR
1	A	448	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	453	ARG
1	A	463	LYS
1	A	464	GLU
1	A	482	LEU
1	A	504	LEU
1	A	507	VAL
1	A	512	LYS
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	575	VAL
1	A	598	LEU
1	A	673	LEU
1	A	688	VAL
1	B	51	ASN
1	B	56	LYS
1	B	57	LEU
1	B	66	HIS
1	B	71	LYS
1	B	96	ASP
1	B	102	ILE
1	B	107	ILE
1	B	129	THR
1	B	137	LEU
1	B	145	GLU
1	B	156	THR
1	B	164	LEU
1	B	180	LEU
1	B	184	ARG
1	B	190	LYS
1	B	202	VAL
1	B	227	GLN
1	B	276	LEU
1	B	313	LEU
1	B	316	LEU
1	B	326	ASP
1	B	343	ARG
1	B	351	THR
1	B	354	VAL
1	B	370	SER
1	B	385	CYS
1	B	388	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	392	LYS
1	B	395	THR
1	B	412	SER
1	B	413	ASP
1	B	448	GLU
1	B	463	LYS
1	B	471	ARG
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	521	GLU
1	B	594	ILE
1	B	597	ARG
1	B	602	GLU
1	B	627	TRP
1	B	658	ARG
1	B	665	VAL
1	B	688	VAL
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	B	764	SER
1	C	61	ARG
1	C	63	ILE
1	C	77	LEU
1	C	129	THR
1	C	140	ARG
1	C	144	THR
1	C	164	LEU
1	C	184	ARG
1	C	239	SER
1	C	246	LEU
1	C	278	SER
1	C	308	GLN
1	C	316	LEU
1	C	323	SER
1	C	326	ASP
1	C	370	SER
1	C	373	LYS
1	C	378	GLU
1	C	379	GLU
1	C	385	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	392	LYS
1	C	413	ASP
1	C	444	CYS
1	C	447	CYS
1	C	452	GLU
1	C	482	LEU
1	C	492	ARG
1	C	504	LEU
1	C	511	SER
1	C	519	LEU
1	C	565	THR
1	C	597	ARG
1	C	598	LEU
1	C	688	VAL
1	D	40	ARG
1	D	41	LYS
1	D	55	LEU
1	D	59	SER
1	D	61	ARG
1	D	66	HIS
1	D	71	LYS
1	D	92	ASN
1	D	94	THR
1	D	96	ASP
1	D	98	PHE
1	D	123	GLN
1	D	129	THR
1	D	164	LEU
1	D	180	LEU
1	D	188	THR
1	D	194	ILE
1	D	227	GLN
1	D	235	LEU
1	D	243	ASP
1	D	276	LEU
1	D	283	THR
1	D	295	ILE
1	D	316	LEU
1	D	323	SER
1	D	326	ASP
1	D	327	ILE
1	D	343	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	350	THR
1	D	354	VAL
1	D	358	ARG
1	D	373	LYS
1	D	385	CYS
1	D	390	ASP
1	D	391	LYS
1	D	392	LYS
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	460	SER
1	D	464	GLU
1	D	482	LEU
1	D	503	MET
1	D	513	LYS
1	D	514	LEU
1	D	519	LEU
1	D	536	LYS
1	D	546	VAL
1	D	575	VAL
1	D	658	ARG
1	D	665	VAL
1	D	711	VAL
1	D	745	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	508	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)

17 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	$\#\|Z\| > 2$
2	NAG	A	1501	1,2	14,14,15	0.63	0	15,19,21	2.14	3 (20%)
2	NAG	A	1502	2	14,14,15	0.53	0	15,19,21	0.85	0
2	NAG	A	1503	1,2	14,14,15	0.64	0	15,19,21	1.56	1 (6%)
2	NAG	A	1504	2	14,14,15	0.68	0	15,19,21	1.48	2 (13%)
2	NAG	A	2291	1,2	14,14,15	0.59	0	15,19,21	0.97	0
2	NAG	A	2292	2	14,14,15	0.60	0	15,19,21	1.43	1 (6%)
2	NAG	A	2811	1,2	14,14,15	0.73	0	15,19,21	1.71	3 (20%)
2	NAG	A	2812	2	14,14,15	0.53	0	15,19,21	0.75	0
2	NAG	B	2291	1,2	14,14,15	0.58	0	15,19,21	1.39	1 (6%)
2	NAG	B	2292	2	14,14,15	0.65	0	15,19,21	1.50	2 (13%)
2	NAG	B	901	1,2	14,14,15	0.56	0	15,19,21	1.23	0
2	NAG	B	902	2	14,14,15	0.48	0	15,19,21	0.89	1 (6%)
5	NAG	C	2291	1,5	14,14,15	0.41	0	15,19,21	1.27	1 (6%)
5	NAG	C	2292	5	14,14,15	0.53	0	15,19,21	3.06	6 (40%)
5	NAG	C	2293	5	14,14,15	0.37	0	15,19,21	1.08	1 (6%)
2	NAG	D	2291	1,2	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
2	NAG	D	2292	2	14,14,15	0.49	0	15,19,21	0.83	0

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	1501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1502	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1503	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2291	1,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2292	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2811	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2812	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2291	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2292	2	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	902	2	-	0/6/23/26	0/1/1/1
5	NAG	C	2291	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2292	5	-	0/6/23/26	0/1/1/1
5	NAG	C	2293	5	-	0/6/23/26	0/1/1/1
2	NAG	D	2291	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2292	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2292	NAG	C4-C3-C2	-5.32	102.97	111.23
2	A	1501	NAG	C4-C3-C2	-3.52	105.75	111.23
5	C	2292	NAG	C3-C4-C5	-2.29	106.20	110.20
5	C	2292	NAG	O7-C7-C8	-2.02	118.35	122.06
2	B	902	NAG	C1-O5-C5	2.02	114.82	112.25
2	D	2291	NAG	C4-C3-C2	2.41	114.97	111.23
2	A	1504	NAG	C3-C4-C5	2.55	114.65	110.20
2	D	2291	NAG	C3-C4-C5	2.55	114.65	110.20
5	C	2292	NAG	C8-C7-N2	2.75	121.37	116.11
2	A	2811	NAG	C3-C4-C5	2.84	115.14	110.20
2	A	2292	NAG	C1-O5-C5	3.00	116.05	112.25
5	C	2293	NAG	C1-O5-C5	3.01	116.07	112.25
2	D	2291	NAG	C1-O5-C5	3.08	116.16	112.25
5	C	2291	NAG	C1-O5-C5	3.10	116.19	112.25
2	B	2292	NAG	C4-C3-C2	3.25	116.28	111.23
2	A	2811	NAG	C1-O5-C5	3.45	116.63	112.25
2	A	1501	NAG	C2-N2-C7	3.49	127.53	123.04
2	A	1504	NAG	C4-C3-C2	3.65	116.91	111.23
2	B	2291	NAG	C1-O5-C5	3.70	116.94	112.25
2	B	2292	NAG	C3-C4-C5	4.12	117.37	110.20
2	A	2811	NAG	C4-C3-C2	4.12	117.64	111.23
2	A	1503	NAG	C2-N2-C7	4.68	129.06	123.04
5	C	2292	NAG	O4-C4-C5	5.31	123.32	109.24
2	A	1501	NAG	C1-O5-C5	5.58	119.33	112.25
5	C	2292	NAG	C1-O5-C5	7.65	121.95	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	901	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2291	NAG	1	0
2	B	2292	NAG	1	0
2	B	901	NAG	1	0
2	B	902	NAG	1	0
5	C	2291	NAG	1	0
2	D	2291	NAG	1	0

5.6 Ligand geometry

16 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	01T	A	1	-	24,27,27	0.44	0	28,39,39	1.69	5 (17%)
3	NAG	A	2191	1	14,14,15	0.57	0	15,19,21	1.48	2 (13%)
3	NAG	A	3211	1	14,14,15	0.57	0	15,19,21	1.60	1 (6%)
4	01T	B	1	-	24,27,27	0.60	0	28,39,39	1.62	4 (14%)
3	NAG	B	1501	1	14,14,15	0.45	0	15,19,21	1.16	1 (6%)
3	NAG	B	2811	1	14,14,15	0.54	0	15,19,21	1.78	1 (6%)
3	NAG	B	3211	1	14,14,15	0.66	0	15,19,21	1.57	4 (26%)
4	01T	C	1	-	24,27,27	0.56	0	28,39,39	1.83	6 (21%)
3	NAG	C	1501	1	14,14,15	0.59	0	15,19,21	2.05	4 (26%)
3	NAG	C	2811	1	14,14,15	0.65	0	15,19,21	1.49	2 (13%)
3	NAG	C	3211	1	14,14,15	0.73	0	15,19,21	1.32	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	01T	D	1	-	24,27,27	0.68	0	28,39,39	1.70	3 (10%)
3	NAG	D	1501	1	14,14,15	0.67	0	15,19,21	2.16	4 (26%)
3	NAG	D	2191	1	14,14,15	0.62	0	15,19,21	1.61	3 (20%)
3	NAG	D	2811	1	14,14,15	0.80	1 (7%)	15,19,21	1.22	2 (13%)
3	NAG	D	5201	1	14,14,15	0.52	0	15,19,21	1.11	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	01T	A	1	-	-	0/14/17/17	0/2/2/2
3	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
3	NAG	A	3211	1	-	0/6/23/26	0/1/1/1
4	01T	B	1	-	-	0/14/17/17	0/2/2/2
3	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2811	1	-	0/6/23/26	0/1/1/1
3	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
4	01T	C	1	-	-	0/14/17/17	0/2/2/2
3	NAG	C	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2811	1	-	0/6/23/26	0/1/1/1
3	NAG	C	3211	1	-	0/6/23/26	0/1/1/1
4	01T	D	1	-	-	0/14/17/17	0/2/2/2
3	NAG	D	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
3	NAG	D	5201	1	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2811	NAG	C1-C2	2.14	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	01T	C15-C3-N4	-5.85	118.58	123.35
4	D	1	01T	C11-C5-N4	-5.28	119.05	123.35
4	A	1	01T	C11-C5-N4	-4.97	119.30	123.35
4	A	1	01T	C15-C3-N4	-4.78	119.46	123.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	01T	C15-C3-N4	-4.68	119.54	123.35
4	B	1	01T	C11-C5-N4	-4.66	119.56	123.35
4	B	1	01T	C15-C3-N4	-4.01	120.08	123.35
4	C	1	01T	C11-C5-N4	-3.66	120.37	123.35
4	C	1	01T	C7-C6-C5	-3.27	111.63	119.26
3	A	2191	NAG	C2-N2-C7	-2.76	119.50	123.04
4	A	1	01T	C7-C6-C5	-2.72	112.90	119.26
4	B	1	01T	C16-C15-C3	-2.71	118.16	120.97
4	C	1	01T	C17-C16-C15	-2.63	111.27	116.31
3	B	3211	NAG	C2-N2-C7	-2.32	120.06	123.04
4	D	1	01T	C7-C6-C5	-2.24	114.04	119.26
4	A	1	01T	C1-C2-C3	-2.21	109.33	115.03
4	B	1	01T	C7-C6-C5	-2.09	114.38	119.26
4	C	1	01T	C21-C20-C26	2.02	121.37	117.55
3	C	1501	NAG	C4-C3-C2	2.03	114.38	111.23
4	C	1	01T	C3-N4-C5	2.11	122.81	118.13
3	C	3211	NAG	C2-N2-C7	2.15	125.80	123.04
4	A	1	01T	C3-N4-C5	2.20	123.01	118.13
3	B	3211	NAG	C3-C4-C5	2.22	114.06	110.20
3	D	1501	NAG	C3-C2-N2	2.28	116.03	110.56
3	C	3211	NAG	C4-C3-C2	2.30	114.80	111.23
3	D	2191	NAG	C3-C4-C5	2.34	114.28	110.20
3	C	1501	NAG	O5-C5-C6	2.38	112.50	107.35
3	D	1501	NAG	O3-C3-C2	2.43	113.93	109.11
3	C	2811	NAG	O5-C5-C6	2.52	112.79	107.35
3	C	1501	NAG	C3-C4-C5	2.75	115.00	110.20
3	B	3211	NAG	C1-O5-C5	2.86	115.88	112.25
3	C	3211	NAG	C1-O5-C5	2.94	115.97	112.25
3	D	2811	NAG	C4-C3-C2	3.07	116.00	111.23
3	D	5201	NAG	C1-O5-C5	3.20	116.31	112.25
3	D	2191	NAG	C4-C3-C2	3.21	116.22	111.23
3	D	2191	NAG	C1-O5-C5	3.26	116.38	112.25
3	D	2811	NAG	C1-O5-C5	3.28	116.41	112.25
3	D	1501	NAG	C2-N2-C7	3.50	127.54	123.04
3	B	1501	NAG	C1-O5-C5	3.73	116.99	112.25
3	B	3211	NAG	C4-C3-C2	3.81	117.15	111.23
3	A	2191	NAG	C1-O5-C5	4.22	117.60	112.25
3	C	2811	NAG	C1-O5-C5	4.62	118.11	112.25
3	A	3211	NAG	C1-O5-C5	5.27	118.94	112.25
3	B	2811	NAG	C1-O5-C5	5.87	119.70	112.25
3	D	1501	NAG	C1-O5-C5	5.91	119.75	112.25
3	C	1501	NAG	C1-O5-C5	6.44	120.42	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	5201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	01T	2	0
4	B	1	01T	1	0
4	D	1	01T	1	0
3	D	2811	NAG	1	0

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	727/740 (98%)	0.29	27 (3%) 45 38	37, 47, 63, 78	0
1	B	733/740 (99%)	0.05	10 (1%) 78 75	35, 47, 61, 80	0
1	C	726/740 (98%)	0.43	60 (8%) 14 9	39, 48, 67, 80	0
1	D	727/740 (98%)	0.31	33 (4%) 37 31	37, 47, 62, 71	0
All	All	2913/2960 (98%)	0.27	130 (4%) 37 31	35, 47, 64, 80	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	ASN	5.9
1	D	87	SER	5.2
1	C	333	SER	5.0
1	C	83	TYR	4.7
1	D	91	GLU	4.5
1	A	88	VAL	4.3
1	D	97	GLU	4.2
1	C	100	HIS	4.1
1	C	412	SER	4.1
1	D	92	ASN	4.0
1	D	72	GLN	3.8
1	C	393	ASP	3.8
1	C	437	SER	3.8
1	A	72	GLN	3.6
1	D	487	ASN	3.6
1	C	487	ASN	3.6
1	D	89	PHE	3.5
1	C	97	GLU	3.5
1	C	440	THR	3.5
1	C	85	ASN	3.4
1	D	279	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	334	SER	3.3
1	C	439	TYR	3.3
1	C	99	GLY	3.2
1	C	338	ASN	3.2
1	D	101	SER	3.2
1	C	392	LYS	3.2
1	D	141	GLN	3.1
1	C	87	SER	3.1
1	C	339	CYS	3.1
1	A	73	GLU	3.1
1	A	97	GLU	3.0
1	A	138	ASN	3.0
1	C	348	MET	3.0
1	C	88	VAL	3.0
1	B	72	GLN	3.0
1	B	34	HIS	2.9
1	C	483	HIS	2.9
1	D	102	ILE	2.9
1	D	88	VAL	2.8
1	C	322	TYR	2.8
1	A	279	VAL	2.8
1	C	438	ASP	2.8
1	C	386	TYR	2.8
1	C	484	SER	2.7
1	A	98	PHE	2.7
1	C	436	LEU	2.7
1	C	342	ALA	2.7
1	C	388	GLN	2.7
1	B	87	SER	2.7
1	D	333	SER	2.7
1	A	76	ILE	2.6
1	A	93	SER	2.6
1	D	75	ASN	2.6
1	D	135	TYR	2.6
1	A	87	SER	2.6
1	C	77	LEU	2.6
1	A	95	PHE	2.5
1	A	99	GLY	2.5
1	A	78	VAL	2.5
1	C	78	VAL	2.5
1	C	468	TYR	2.5
1	C	135	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	467	TYR	2.5
1	D	489	LYS	2.5
1	D	85	ASN	2.5
1	C	98	PHE	2.5
1	A	75	ASN	2.5
1	C	442	VAL	2.5
1	A	506	ASN	2.4
1	D	100	HIS	2.4
1	C	335	GLY	2.4
1	C	448	GLU	2.4
1	D	83	TYR	2.4
1	C	390	ASP	2.4
1	A	92	ASN	2.4
1	C	222	PHE	2.4
1	A	140	ARG	2.4
1	D	73	GLU	2.4
1	D	467	TYR	2.4
1	A	74	ASN	2.4
1	B	734	TRP	2.3
1	C	67	GLU	2.3
1	C	277	SER	2.3
1	C	397	ILE	2.3
1	D	336	ARG	2.3
1	C	72	GLN	2.3
1	C	285	ILE	2.3
1	B	83	TYR	2.3
1	C	82	GLU	2.3
1	C	178	PRO	2.3
1	D	140	ARG	2.2
1	C	432	TYR	2.2
1	D	277	SER	2.2
1	A	652	ALA	2.2
1	C	183	TYR	2.2
1	C	414	TYR	2.2
1	A	704	HIS	2.2
1	D	77	LEU	2.2
1	B	333	SER	2.2
1	D	79	PHE	2.2
1	A	636	THR	2.2
1	B	733	MET	2.2
1	C	464	GLU	2.2
1	D	144	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	SER	2.1
1	C	280	THR	2.1
1	C	400	GLY	2.1
1	C	435	GLN	2.1
1	A	333	SER	2.1
1	A	392	LYS	2.1
1	B	88	VAL	2.1
1	D	392	LYS	2.1
1	C	415	LEU	2.1
1	B	70	TYR	2.1
1	D	95	PHE	2.1
1	A	141	GLN	2.1
1	A	655	PRO	2.1
1	A	732	ALA	2.1
1	C	179	ASN	2.1
1	C	488	ASP	2.1
1	A	135	TYR	2.1
1	D	142	LEU	2.1
1	C	350	THR	2.0
1	C	394	CYS	2.0
1	D	187	TRP	2.0
1	D	99	GLY	2.0
1	C	413	ASP	2.0
1	C	482	LEU	2.0
1	C	766	PRO	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)

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	D	2291	14/15	0.90	0.22	0.65	60,63,67,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	2291	14/15	0.93	0.21	-0.08	55,57,59,61	0
2	NAG	B	2291	14/15	0.89	0.17	-0.95	58,61,63,67	0
2	NAG	A	1503	14/15	0.79	0.19	-1.33	86,88,90,92	0
5	NAG	C	2291	14/15	0.93	0.14	-1.42	60,63,65,68	0
2	NAG	A	1504	14/15	0.74	0.33	-	94,94,96,96	0
2	NAG	A	2811	14/15	0.74	0.18	-	64,68,70,73	0
2	NAG	B	2292	14/15	0.82	0.31	-	71,72,73,73	0
2	NAG	D	2292	14/15	0.80	0.32	-	74,76,79,80	0
2	NAG	A	2292	14/15	0.74	0.32	-	61,63,65,66	0
5	NAG	C	2292	14/15	0.84	0.21	-	70,73,76,80	0
2	NAG	A	1502	14/15	0.79	0.40	-	86,88,89,89	0
5	NAG	C	2293	14/15	0.76	0.26	-	83,85,87,88	0
2	NAG	A	2812	14/15	0.82	0.26	-	76,78,78,78	0
2	NAG	B	902	14/15	0.75	0.33	-	95,97,97,97	0
2	NAG	A	1501	14/15	0.81	0.32	-	73,78,80,84	0
2	NAG	B	901	14/15	0.69	0.20	-	87,89,91,93	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, 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
3	NAG	D	5201	14/15	0.67	0.35	16.26	75,78,81,82	0
3	NAG	B	3211	14/15	0.80	0.42	7.21	59,62,63,63	0
3	NAG	A	3211	14/15	0.86	0.27	1.62	55,57,62,62	0
4	01T	B	1	26/26	0.95	0.28	0.90	45,48,51,55	0
4	01T	D	1	26/26	0.94	0.25	0.59	45,48,55,58	0
3	NAG	C	3211	14/15	0.71	0.29	0.40	66,69,75,76	0
4	01T	A	1	26/26	0.95	0.29	0.39	46,49,56,59	0
4	01T	C	1	26/26	0.95	0.21	0.33	44,47,50,51	0
3	NAG	D	2811	14/15	0.80	0.19	-	63,65,67,67	0
3	NAG	D	1501	14/15	0.75	0.28	-	63,66,66,66	0
3	NAG	A	2191	14/15	0.78	0.36	-	61,65,70,70	0
3	NAG	C	2811	14/15	0.91	0.15	-	63,65,67,67	0
3	NAG	B	1501	14/15	0.88	0.23	-	61,62,63,64	0
3	NAG	D	2191	14/15	0.87	0.29	-	60,64,67,68	0
3	NAG	C	1501	14/15	0.82	0.19	-	64,66,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	2811	14/15	0.88	0.12	-	57,59,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.