



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G0D  
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 2  
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.  
Deposited on : 2009-01-27  
Resolution : 2.39 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](mailto: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

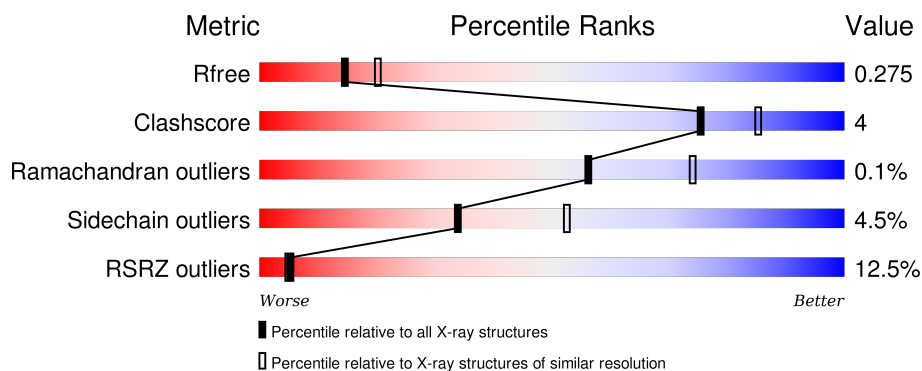
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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	740	<div> <div>9%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	B	740	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	740	<div> <div>13%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	D	740	<div> <div>20%</div> <div>85%</div> <div>11%</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	C	806	-	-	-	X
3	NAG	D	804	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25530 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	723	Total	C	N	O	S	0	3	0
			5936	3813	977	1120	26			
1	B	728	Total	C	N	O	S	0	3	0
			5970	3833	985	1126	26			
1	C	723	Total	C	N	O	S	0	1	0
			5927	3808	975	1118	26			
1	D	723	Total	C	N	O	S	0	0	0
			5918	3800	973	1119	26			

There are 48 discrepancies between the modelled and reference sequences:

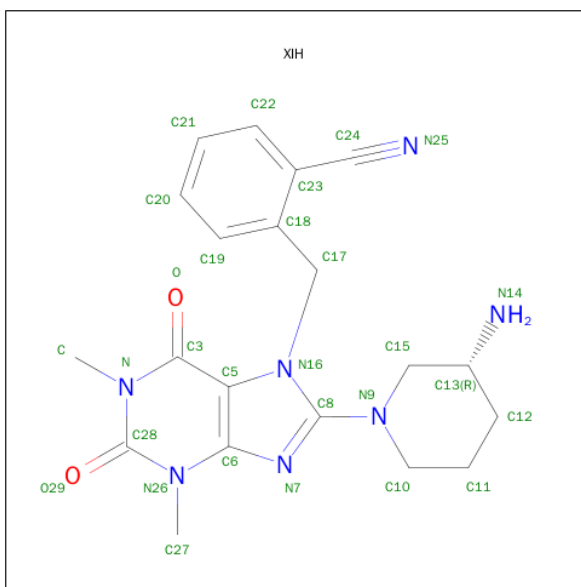
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
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...*

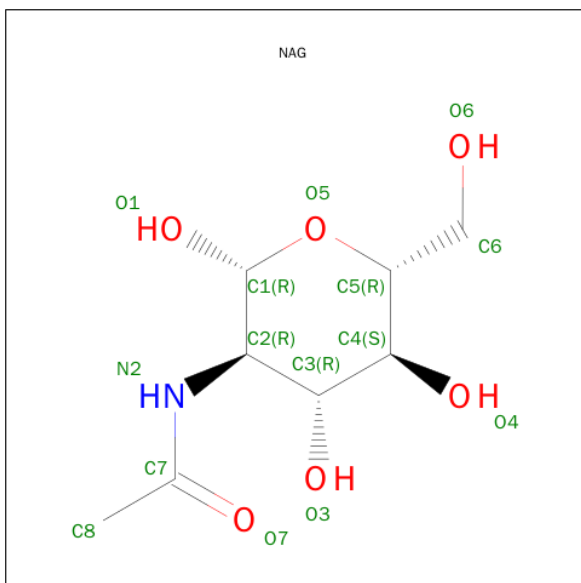
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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 2-({8-[(3R)-3-AMINOPIPERIDIN-1-YL]-1,3-DIMETHYL-2,6-DIOXO-1,2,3,6-TETRAHYDRO-7H-PURIN-7-YL}METHYL)BENZONITRILE (three-letter code: XIH) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	7	2		
2	B	1	Total	C	N	O	0	0
			29	20	7	2		
2	C	1	Total	C	N	O	0	0
			29	20	7	2		
2	D	1	Total	C	N	O	0	0
			29	20	7	2		

- 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	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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	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	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is water.

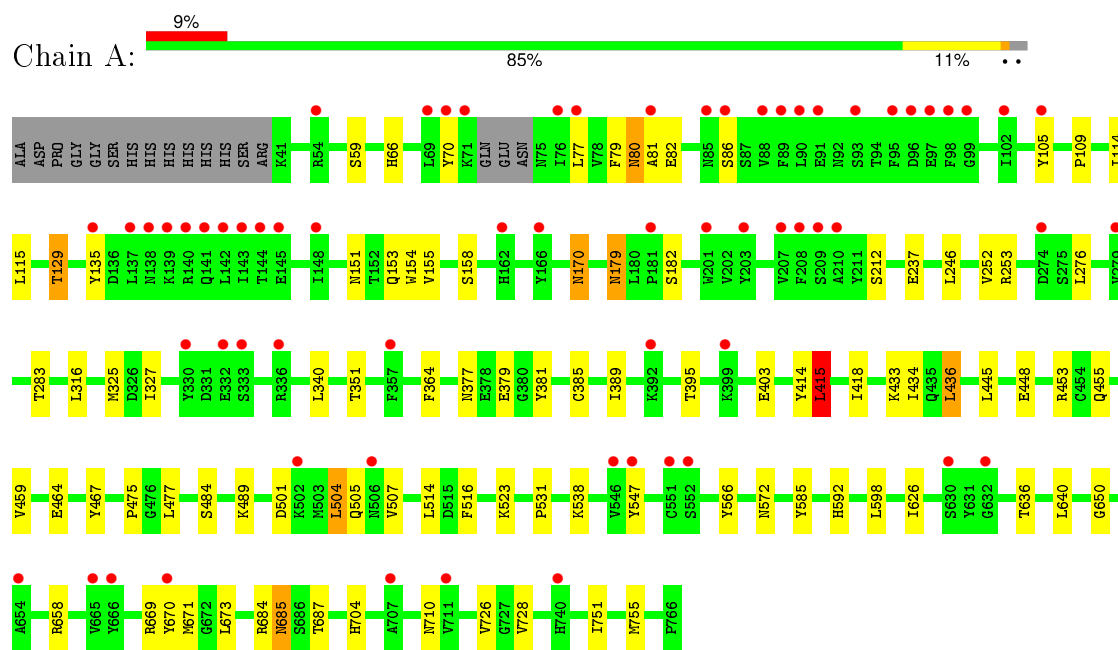
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	394	Total 394	O 394	0	0
5	B	370	Total 370	O 370	0	0
5	C	348	Total 348	O 348	0	0
5	D	215	Total 215	O 215	0	0



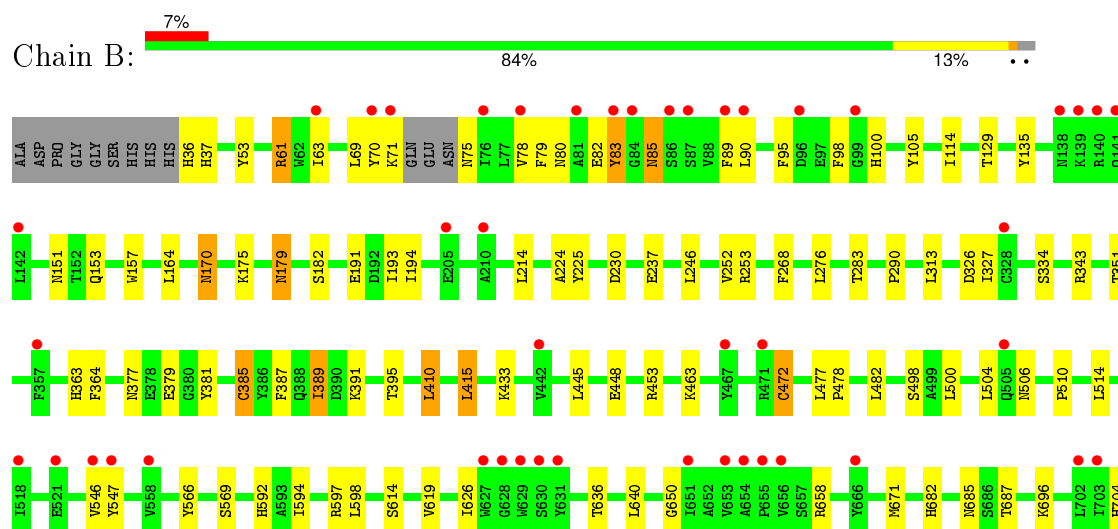
### 3 Residue-property plots [i](#)

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

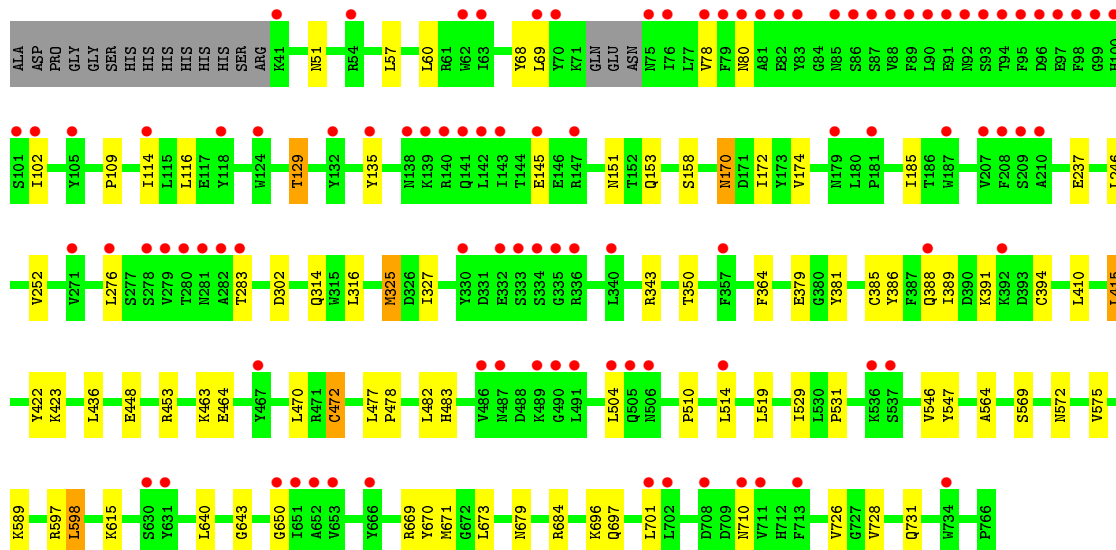
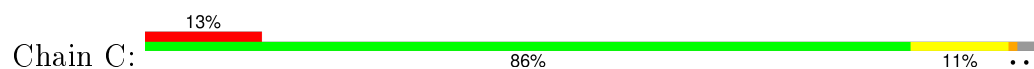


#### • Molecule 1: Dipeptidyl peptidase 4

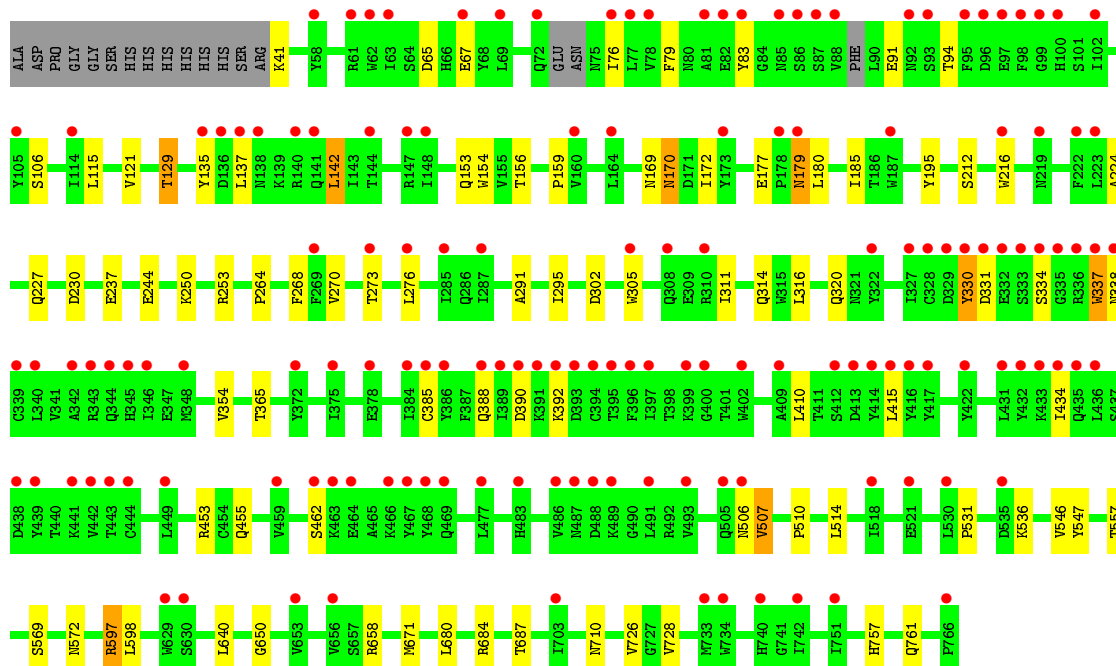
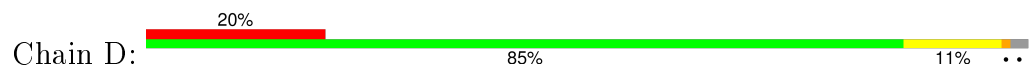




• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.91Å 123.44Å 145.68Å 90.00° 114.69° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 48.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.39) 95.2 (48.71-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.239 0.232 , 0.275	Depositor DCC
$R_{free}$ test set	7412 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.6	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 147788 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: XIH, 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	0.45	0/6119	0.60	1/8321 (0.0%)
1	B	0.45	0/6155	0.59	1/8370 (0.0%)
1	C	0.45	0/6102	0.60	1/8298 (0.0%)
1	D	0.48	4/6087 (0.1%)	0.58	4/8277 (0.0%)
All	All	0.45	4/24463 (0.0%)	0.59	7/33266 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	ASN	CG-OD1	11.25	1.48	1.24
1	D	337	TRP	CD2-CE2	6.56	1.49	1.41
1	D	338	ASN	C-O	6.05	1.34	1.23
1	D	270	VAL	CB-CG1	5.74	1.65	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	D	330	TYR	CB-CG-CD2	8.35	126.01	121.00
1	B	415	LEU	CA-CB-CG	6.19	129.53	115.30
1	C	415	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	415	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	142	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	330	TYR	O-C-N	5.12	130.89	122.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5936	0	5655	55	0
1	B	5970	0	5678	53	0
1	C	5927	0	5650	40	0
1	D	5918	0	5641	38	0
2	A	29	0	23	0	0
2	B	29	0	23	1	0
2	C	29	0	23	0	0
2	D	29	0	23	0	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	56	0	52	0	0
3	D	28	0	26	0	0
4	A	56	0	50	0	0
4	B	28	0	25	0	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
5	A	394	0	0	2	0
5	B	370	0	0	1	0
5	C	348	0	0	1	0
5	D	215	0	0	1	0
All	All	25530	0	23023	186	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 4.

All (186) 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:A:153:GLN:HE22	1:A:170:ASN:H	1.11	0.91
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.20	0.90
1:C:153:GLN:HE22	1:C:170:ASN:H	1.19	0.89
1:B:379:GLU:HG3	1:B:381:TYR:HD1	1.39	0.87
1:B:36:HIS:CD2	1:B:37:HIS:H	1.95	0.85
1:B:153:GLN:HE22	1:B:170:ASN:H	1.26	0.84
1:D:153:GLN:HE22	1:D:170:ASN:H	1.29	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.23	0.73
1:B:731[B]:GLN:HG3	5:B:1227:HOH:O	1.90	0.71
1:A:129:THR:HG23	1:A:151:ASN:HA	1.73	0.69
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.75	0.69
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.75	0.68
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.77	0.67
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.75	0.66
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.76	0.66
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.79	0.65
1:C:564:ALA:HB1	1:C:575:VAL:HG11	1.79	0.64
1:B:129:THR:HG23	1:B:151:ASN:HA	1.80	0.63
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.82	0.61
1:B:379:GLU:HG3	1:B:381:TYR:CD1	2.29	0.60
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.65	0.60
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.85	0.59
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.85	0.59
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.86	0.58
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.85	0.58
1:C:388:GLN:HG3	1:C:391:LYS:HE3	1.86	0.58
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.87	0.57
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.40	0.56
1:A:179:ASN:H	1:A:179:ASN:HD22	1.52	0.56
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.87	0.55
1:C:529:ILE:HB	1:C:575:VAL:HG13	1.89	0.55
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.87	0.55
1:A:379:GLU:HG3	1:A:381:TYR:HD1	1.70	0.55
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.37	0.55
1:D:598:LEU:HD22	1:D:671:MET:HG2	1.88	0.55
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.88	0.54
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.89	0.54
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.72	0.54
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.89	0.54
1:C:379:GLU:HG3	1:C:381:TYR:HD1	1.71	0.54
1:B:71:LYS:HG3	1:B:75:ASN:HB3	1.90	0.54
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.91	0.53
1:D:195:TYR:O	1:D:227:GLN:HA	2.08	0.53
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.74	0.53
1:D:273:THR:HA	1:D:276:LEU:HD13	1.91	0.53
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.91	0.53
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.91	0.53
1:A:598:LEU:HB2	1:A:671:MET:SD	2.50	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ARG:HD2	1:C:389:ILE:HG23	1.91	0.52
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.92	0.52
1:A:80:ASN:HD22	1:A:82:GLU:H	1.58	0.52
1:D:291:ALA:O	1:D:295:ILE:HG23	2.09	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.44	0.52
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.92	0.52
1:B:614:SER:HA	1:B:619:VAL:HB	1.92	0.51
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.76	0.51
1:D:415:LEU:HB3	1:D:434:ILE:HG23	1.93	0.51
1:B:377:ASN:OD1	1:B:379:GLU:HG2	2.11	0.51
1:A:179:ASN:N	1:A:179:ASN:HD22	2.07	0.51
1:D:177:GLU:HB2	1:D:180:LEU:HG	1.92	0.51
1:C:153:GLN:NE2	1:C:170:ASN:H	1.99	0.51
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.75	0.51
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.46	0.50
1:A:59:SER:O	1:A:70:TYR:HD1	1.93	0.50
1:D:121:VAL:HB	1:D:129:THR:HG22	1.92	0.50
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.46	0.50
1:B:179:ASN:H	1:B:179:ASN:HD22	1.60	0.50
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.95	0.49
1:C:597:ARG:NH1	1:C:679:ASN:OD1	2.46	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.92	0.49
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.43	0.49
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.95	0.49
1:C:172:ILE:HG22	1:C:185:ILE:HD12	1.94	0.49
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.96	0.49
1:A:684[B]:ARG:HD2	5:A:982:HOH:O	2.12	0.49
1:A:325:MET:CE	1:A:327:ILE:HD11	2.42	0.48
1:C:69:LEU:HD23	1:C:78:VAL:HG22	1.95	0.48
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.48	0.48
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.79	0.48
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.94	0.48
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.96	0.48
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.95	0.48
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.79	0.48
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.78	0.48
1:A:77:LEU:HB3	1:A:86:SER:HB2	1.96	0.47
2:B:800:XIH:H101	2:B:800:XIH:H172	1.96	0.47
1:B:80:ASN:HB3	1:B:85:ASN:O	2.15	0.47
1:D:757:HIS:HD2	5:D:1339:HOH:O	1.97	0.47
1:D:91:GLU:HB3	1:D:94:THR:OG1	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:N	1:A:170:ASN:HD22	2.12	0.47
1:C:170:ASN:N	1:C:170:ASN:HD22	2.13	0.47
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.79	0.47
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.97	0.47
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.79	0.47
1:C:129:THR:HG23	1:C:151:ASN:HA	1.96	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.50	0.46
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.97	0.46
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.97	0.46
1:C:684[A]:ARG:HD2	5:C:1004:HOH:O	2.15	0.46
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.98	0.46
1:D:179:ASN:ND2	1:D:179:ASN:H	2.11	0.46
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.98	0.46
1:A:467:TYR:HD2	1:A:484:SER:HA	1.81	0.46
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.80	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.44	0.46
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.46
1:B:433:LYS:HD2	1:B:445:LEU:HD21	1.98	0.46
1:A:237:GLU:HA	1:A:252:VAL:O	2.16	0.45
1:A:377:ASN:OD1	1:A:379:GLU:HG2	2.15	0.45
1:A:414:TYR:CD2	1:A:433:LYS:HD3	2.51	0.45
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.99	0.45
1:B:290:PRO:HD3	1:B:326:ASP:OD1	2.16	0.45
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.50	0.45
1:A:501:ASP:O	1:A:505[B]:GLN:HG2	2.17	0.45
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.47	0.45
1:D:67:GLU:HA	1:D:79:PHE:O	2.17	0.45
1:B:36:HIS:CG	1:B:37:HIS:H	2.32	0.45
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.99	0.45
1:D:320:GLN:O	1:D:354:VAL:HG12	2.17	0.45
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.99	0.44
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.99	0.44
1:B:710:ASN:C	1:B:710:ASN:HD22	2.20	0.44
1:A:179:ASN:H	1:A:179:ASN:ND2	2.15	0.44
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.98	0.44
1:A:80:ASN:HD22	1:A:81:ALA:N	2.15	0.44
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.18	0.44
1:A:467:TYR:CD2	1:A:484:SER:HA	2.53	0.44
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ILE:H	1:D:91:GLU:HA	1.83	0.43
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.99	0.43
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.53	0.43
1:D:135:TYR:CZ	1:D:142:LEU:HB2	2.53	0.43
1:A:66:HIS:HB3	1:A:467:TYR:HE1	1.82	0.43
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.53	0.43
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.53	0.43
1:A:685:ASN:ND2	5:A:981:HOH:O	2.51	0.43
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.99	0.43
1:A:415:LEU:HB2	1:A:436:LEU:HD11	2.00	0.43
1:D:597:ARG:HA	1:D:597:ARG:HD3	1.84	0.43
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.99	0.43
1:B:598:LEU:O	1:B:682:HIS:NE2	2.48	0.43
1:B:598:LEU:HB2	1:B:671:MET:SD	2.59	0.43
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.43
1:B:626:ILE:O	1:B:650:GLY:HA2	2.18	0.43
1:D:156:THR:HG23	1:D:216:TRP:HE1	1.83	0.43
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.49	0.42
1:A:109:PRO:HG2	1:A:158:SER:O	2.18	0.42
1:B:61:ARG:HG3	1:B:69:LEU:HB2	2.02	0.42
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.34	0.42
1:A:751:ILE:O	1:A:755:MET:HG3	2.19	0.42
1:B:327:ILE:HD13	1:B:389:ILE:HG13	2.00	0.42
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.35	0.42
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.19	0.42
1:A:418:ILE:HD11	1:A:459:VAL:HG12	2.02	0.42
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.42
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.54	0.41
1:A:153:GLN:HE22	1:A:170:ASN:N	1.95	0.41
1:B:191:GLU:O	1:B:193:ILE:HD12	2.20	0.41
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.03	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:A:504:LEU:HA	1:A:507:VAL:HG12	2.02	0.41
1:B:363:HIS:HB3	1:B:410:LEU:HD22	2.02	0.41
1:D:65:ASP:HA	1:D:462:SER:HB2	2.02	0.41
1:D:169:ASN:O	1:D:170:ASN:HB2	2.21	0.41
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.55	0.41
1:B:53:TYR:HB3	1:B:500:LEU:HD11	2.03	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.20	0.41
1:C:102:ILE:HD12	1:C:116:LEU:HB3	2.03	0.41
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.86	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.40
1:C:386:TYR:O	1:C:394:CYS:HB2	2.21	0.40
1:C:109:PRO:HG2	1:C:158:SER:O	2.21	0.40
1:B:82:GLU:HB2	1:B:83:TYR:CD1	2.56	0.40
1:B:237:GLU:HA	1:B:252:VAL:O	2.22	0.40
1:D:41:LYS:HG3	1:D:507:VAL:HG12	2.03	0.40
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.56	0.40
1:D:680:LEU:O	1:D:684:ARG:HG3	2.21	0.40
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.03	0.40
1:B:658:ARG:HB2	1:B:687:THR:HG22	2.03	0.40
1:C:60:LEU:HB2	1:C:68:TYR:CD1	2.56	0.40
1:C:510:PRO:HD3	1:C:569:SER:HB2	2.04	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	722/740 (98%)	690 (96%)	32 (4%)	0	100	100
1	B	727/740 (98%)	702 (97%)	24 (3%)	1 (0%)	56	74
1	C	720/740 (97%)	692 (96%)	28 (4%)	0	100	100
1	D	717/740 (97%)	687 (96%)	29 (4%)	1 (0%)	56	74
All	All	2886/2960 (98%)	2771 (96%)	113 (4%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	LYS
1	D	390	ASP

### 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	651/662 (98%)	623 (96%)	28 (4%)	35	55
1	B	654/662 (99%)	620 (95%)	34 (5%)	29	45
1	C	649/662 (98%)	616 (95%)	33 (5%)	29	46
1	D	648/662 (98%)	625 (96%)	23 (4%)	43	64
All	All	2602/2648 (98%)	2484 (96%)	118 (4%)	34	52

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	129	THR
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	340	LEU
1	A	385	CYS
1	A	395	THR
1	A	415	LEU
1	A	436	LEU
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	477	LEU
1	A	489	LYS
1	A	504	LEU
1	A	514	LEU
1	A	538	LYS
1	A	547	TYR
1	A	566	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	673	LEU
1	A	685	ASN
1	A	704	HIS
1	A	710	ASN
1	B	61	ARG
1	B	63	ILE
1	B	83	TYR
1	B	85	ASN
1	B	170	ASN
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	334	SER
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	448	GLU
1	B	453	ARG
1	B	472	CYS
1	B	477	LEU
1	B	482	LEU
1	B	498	SER
1	B	504	LEU
1	B	506	ASN
1	B	514	LEU
1	B	546	VAL
1	B	547	TYR
1	B	566	TYR
1	B	594	ILE
1	B	685	ASN
1	B	704	HIS
1	B	710	ASN
1	C	51	ASN
1	C	57	LEU
1	C	80	ASN
1	C	129	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	145	GLU
1	C	170	ASN
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET
1	C	350	THR
1	C	385	CYS
1	C	410	LEU
1	C	415	LEU
1	C	436	LEU
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	464	GLU
1	C	472	CYS
1	C	477	LEU
1	C	482	LEU
1	C	504	LEU
1	C	514	LEU
1	C	519	LEU
1	C	546	VAL
1	C	547	TYR
1	C	589	LYS
1	C	598	LEU
1	C	615	LYS
1	C	673	LEU
1	C	710	ASN
1	D	83	TYR
1	D	129	THR
1	D	137	LEU
1	D	170	ASN
1	D	179	ASN
1	D	244	GLU
1	D	250	LYS
1	D	316	LEU
1	D	365	THR
1	D	385	CYS
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	453	ARG
1	D	506	ASN
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	546	VAL
1	D	547	TYR
1	D	597	ARG
1	D	710	ASN
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	141	GLN
1	A	151	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	B	36	HIS
1	B	80	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	80	ASN
1	C	123	GLN
1	C	153	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	572	ASN
1	C	685	ASN
1	C	694	ASN
1	C	697	GLN
1	C	710	ASN
1	D	75	ASN
1	D	112	GLN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS
1	D	685	ASN
1	D	710	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 ⓘ

10 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
4	NAG	A	804	1,4	14,14,15	0.64	0	15,19,21	0.86	0
4	NAG	A	805	4	14,14,15	0.43	0	15,19,21	1.12	1 (6%)
4	NAG	A	806	1,4	14,14,15	0.48	0	15,19,21	1.12	1 (6%)
4	NAG	A	807	4	14,14,15	0.50	0	15,19,21	0.68	0
4	NAG	B	804	1,4	14,14,15	0.57	0	15,19,21	0.80	0
4	NAG	B	805	4	14,14,15	0.50	0	15,19,21	1.44	1 (6%)
4	NAG	C	803	1,4	14,14,15	0.59	0	15,19,21	0.99	1 (6%)
4	NAG	C	804	4	14,14,15	0.48	0	15,19,21	0.66	0
4	NAG	D	802	1,4	14,14,15	0.47	0	15,19,21	0.91	1 (6%)
4	NAG	D	803	4	14,14,15	0.45	0	15,19,21	1.06	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	A	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	805	4	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	807	4	-	0/6/23/26	0/1/1/1
4	NAG	B	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	4	-	0/6/23/26	0/1/1/1
4	NAG	C	803	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	804	4	-	0/6/23/26	0/1/1/1
4	NAG	D	802	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	803	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	NAG	C4-C3-C2	2.08	114.46	111.23
4	D	802	NAG	C1-O5-C5	2.17	115.01	112.25
4	D	803	NAG	C1-O5-C5	2.79	115.78	112.25
4	A	806	NAG	C1-O5-C5	2.87	115.89	112.25
4	A	805	NAG	C1-O5-C5	3.53	116.73	112.25
4	B	805	NAG	C1-O5-C5	4.96	118.54	112.25

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	XIH	A	800	-	25,32,32	2.34	4 (16%)	26,47,47	2.07	6 (23%)
3	NAG	A	801	1	14,14,15	0.50	0	15,19,21	0.86	1 (6%)
3	NAG	A	802	1	14,14,15	0.50	0	15,19,21	0.99	1 (6%)
3	NAG	A	803	1	14,14,15	0.51	0	15,19,21	0.85	0
3	NAG	A	808	1	14,14,15	0.53	0	15,19,21	1.14	1 (6%)
2	XIH	B	800	-	25,32,32	2.37	4 (16%)	26,47,47	2.06	8 (30%)
3	NAG	B	801	1	14,14,15	0.67	0	15,19,21	1.27	2 (13%)
3	NAG	B	802	1	14,14,15	0.51	0	15,19,21	1.61	1 (6%)
3	NAG	B	803	1	14,14,15	0.59	0	15,19,21	0.99	1 (6%)
3	NAG	B	806	1	14,14,15	0.49	0	15,19,21	1.58	3 (20%)
2	XIH	C	800	-	25,32,32	2.54	5 (20%)	26,47,47	2.01	9 (34%)
3	NAG	C	801	1	14,14,15	0.61	0	15,19,21	1.14	1 (6%)
3	NAG	C	802	1	14,14,15	0.58	0	15,19,21	0.98	1 (6%)
3	NAG	C	805	1	14,14,15	0.60	0	15,19,21	1.16	1 (6%)
3	NAG	C	806	1	14,14,15	0.51	0	15,19,21	0.94	1 (6%)
2	XIH	D	800	-	25,32,32	2.57	4 (16%)	26,47,47	1.76	4 (15%)
3	NAG	D	801	1	14,14,15	0.54	0	15,19,21	1.02	1 (6%)
3	NAG	D	804	1	14,14,15	0.60	0	15,19,21	1.38	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XIH	A	800	-	-	0/6/20/20	0/4/4/4
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	XIH	B	800	-	-	0/6/20/20	0/4/4/4
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
2	XIH	C	800	-	-	0/6/20/20	0/4/4/4
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	805	1	-	0/6/23/26	0/1/1/1
3	NAG	C	806	1	-	0/6/23/26	0/1/1/1
2	XIH	D	800	-	-	0/6/20/20	0/4/4/4
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	XIH	C23-C24	-10.21	1.29	1.44
2	D	800	XIH	C23-C24	-10.19	1.29	1.44
2	B	800	XIH	C23-C24	-9.55	1.30	1.44
2	A	800	XIH	C23-C24	-9.24	1.30	1.44
2	D	800	XIH	C6-N26	-4.44	1.34	1.39
2	B	800	XIH	C6-N26	-4.22	1.34	1.39
2	A	800	XIH	C6-N26	-3.90	1.34	1.39
2	C	800	XIH	C6-N26	-3.61	1.35	1.39
2	B	800	XIH	C3-N	2.16	1.41	1.38
2	C	800	XIH	C6-N7	2.24	1.35	1.33
2	C	800	XIH	C3-N	2.69	1.42	1.38
2	A	800	XIH	C3-N	2.76	1.42	1.38
2	D	800	XIH	C3-N	3.43	1.43	1.38
2	B	800	XIH	C3-C5	3.65	1.47	1.41
2	C	800	XIH	C3-C5	4.23	1.48	1.41
2	A	800	XIH	C3-C5	4.49	1.49	1.41
2	D	800	XIH	C3-C5	4.71	1.49	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	XIH	C3-C5-C6	-3.67	117.30	119.93
2	C	800	XIH	C11-C12-C13	-3.07	107.73	111.97
2	D	800	XIH	C3-C5-C6	-2.75	117.96	119.93
2	C	800	XIH	C17-C18-C19	-2.66	114.99	121.09
2	C	800	XIH	C3-C5-C6	-2.63	118.05	119.93
2	A	800	XIH	C17-C18-C19	-2.50	115.36	121.09
3	B	806	NAG	C4-C3-C2	-2.28	107.68	111.23
2	B	800	XIH	C3-C5-C6	-2.19	118.36	119.93
2	B	800	XIH	C17-C18-C19	-2.17	116.12	121.09
3	B	806	NAG	C3-C4-C5	-2.05	106.63	110.20
3	C	806	NAG	C1-O5-C5	2.05	114.85	112.25
3	C	802	NAG	C4-C3-C2	2.07	114.44	111.23
3	D	801	NAG	C1-O5-C5	2.14	114.96	112.25
2	C	800	XIH	C12-C11-C10	2.15	113.84	110.97
2	B	800	XIH	C11-C10-N9	2.16	115.35	111.17
2	B	800	XIH	C27-N26-C6	2.18	121.65	118.39
2	C	800	XIH	C19-C18-C23	2.21	120.36	117.79
3	B	803	NAG	C1-O5-C5	2.34	115.21	112.25
3	A	801	NAG	C1-O5-C5	2.47	115.39	112.25
2	D	800	XIH	C17-C18-C23	2.48	123.55	120.26
3	B	801	NAG	O5-C5-C6	2.75	113.30	107.35
3	D	804	NAG	C4-C3-C2	2.78	115.55	111.23
3	C	801	NAG	C1-O5-C5	2.82	115.82	112.25
2	C	800	XIH	C18-C23-C24	2.84	122.56	120.10
3	B	801	NAG	C4-C3-C2	3.05	115.97	111.23
3	D	804	NAG	C1-O5-C5	3.06	116.13	112.25
3	C	805	NAG	C1-O5-C5	3.07	116.15	112.25
3	A	802	NAG	C1-O5-C5	3.20	116.31	112.25
2	C	800	XIH	C17-C18-C23	3.25	124.59	120.26
2	A	800	XIH	C17-C18-C23	3.27	124.61	120.26
2	B	800	XIH	C17-C18-C23	3.36	124.72	120.26
3	A	808	NAG	C1-O5-C5	3.60	116.81	112.25
2	A	800	XIH	C18-C23-C24	3.83	123.41	120.10
2	A	800	XIH	C18-C17-N16	3.90	119.78	113.31
2	B	800	XIH	C18-C23-C24	3.95	123.52	120.10
2	B	800	XIH	C18-C17-N16	3.95	119.87	113.31
2	D	800	XIH	C18-C17-N16	4.03	120.00	113.31
3	B	806	NAG	C1-O5-C5	4.25	117.64	112.25
2	C	800	XIH	C18-C17-N16	4.44	120.68	113.31
2	C	800	XIH	C10-N9-C15	4.85	123.47	113.30
3	B	802	NAG	C1-O5-C5	5.22	118.88	112.25
2	D	800	XIH	C10-N9-C15	5.26	124.33	113.30
2	A	800	XIH	C10-N9-C15	5.32	124.45	113.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	XIH	C10-N9-C15	5.40	124.64	113.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	804	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	XIH	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	723/740 (97%)	0.71	65 (8%) 12 11	39, 48, 74, 104	0
1	B	728/740 (98%)	0.55	51 (7%) 19 19	36, 49, 72, 93	0
1	C	723/740 (97%)	0.81	97 (13%) 4 4	39, 49, 73, 93	0
1	D	723/740 (97%)	1.15	149 (20%) 1 1	38, 54, 82, 118	0
All	All	2897/2960 (97%)	0.80	362 (12%) 5 5	36, 50, 76, 118	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	7.8
1	A	81	ALA	7.7
1	D	77	LEU	7.4
1	D	92	ASN	7.3
1	C	279	VAL	7.2
1	B	81	ALA	7.1
1	D	322	TYR	6.6
1	C	89	PHE	6.5
1	D	467	TYR	5.9
1	D	415	LEU	5.9
1	A	86	SER	5.8
1	C	83	TYR	5.7
1	D	333	SER	5.6
1	A	95	PHE	5.6
1	D	416	TYR	5.5
1	C	93	SER	5.5
1	D	372	TYR	5.5
1	A	135	TYR	5.4
1	D	396	PHE	5.3
1	C	88	VAL	5.3
1	D	97	GLU	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	397	ILE	5.3
1	C	76	ILE	5.3
1	D	135	TYR	5.2
1	D	81	ALA	5.2
1	B	78	VAL	5.2
1	D	386	TYR	5.1
1	D	98	PHE	5.1
1	D	148	ILE	5.0
1	D	464	GLU	5.0
1	D	93	SER	5.0
1	D	138	ASN	5.0
1	D	141	GLN	4.9
1	C	97	GLU	4.9
1	A	90	LEU	4.9
1	C	90	LEU	4.8
1	D	391	LYS	4.8
1	D	62	TRP	4.8
1	C	87	SER	4.8
1	D	468	TYR	4.8
1	D	335	GLY	4.7
1	D	78	VAL	4.7
1	D	442	VAL	4.7
1	D	392	LYS	4.6
1	A	93	SER	4.6
1	C	330	TYR	4.5
1	C	96	ASP	4.5
1	A	140	ARG	4.5
1	C	95	PHE	4.5
1	A	141	GLN	4.4
1	C	98	PHE	4.4
1	D	140	ARG	4.4
1	D	330	TYR	4.4
1	D	414	TYR	4.3
1	A	332	GLU	4.3
1	D	389	ILE	4.3
1	C	138	ASN	4.3
1	B	70	TYR	4.3
1	D	105	TYR	4.3
1	A	88	VAL	4.2
1	D	395	THR	4.1
1	D	332	GLU	4.1
1	C	86	SER	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	137	LEU	4.1
1	D	339	CYS	4.1
1	D	491	LEU	4.1
1	D	439	TYR	4.1
1	D	222	PHE	4.0
1	C	78	VAL	4.0
1	D	88	VAL	4.0
1	C	467	TYR	4.0
1	D	83	TYR	3.9
1	D	102	ILE	3.9
1	D	449	LEU	3.8
1	D	375	ILE	3.8
1	D	417	TYR	3.8
1	D	338	ASN	3.8
1	A	76	ILE	3.8
1	C	486	VAL	3.8
1	B	89	PHE	3.7
1	D	483	HIS	3.7
1	D	82	GLU	3.7
1	D	348	MET	3.7
1	A	97	GLU	3.7
1	C	85	ASN	3.7
1	A	70	TYR	3.7
1	A	139	LYS	3.6
1	C	141	GLN	3.6
1	A	96	ASP	3.6
1	A	98	PHE	3.6
1	A	99	GLY	3.5
1	A	91	GLU	3.5
1	C	101	SER	3.5
1	D	432	TYR	3.5
1	A	138	ASN	3.5
1	D	346	ILE	3.5
1	D	100	HIS	3.5
1	D	331	ASP	3.5
1	D	463	LYS	3.4
1	D	433	LYS	3.4
1	D	276	LEU	3.4
1	D	345	HIS	3.4
1	A	89	PHE	3.4
1	C	92	ASN	3.4
1	D	67	GLU	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	83	TYR	3.4
1	D	76	ILE	3.4
1	D	436	LEU	3.4
1	D	87	SER	3.4
1	D	518	ILE	3.4
1	D	385	CYS	3.3
1	A	279	VAL	3.3
1	A	333	SER	3.3
1	D	58	TYR	3.3
1	B	629	TRP	3.3
1	C	100	HIS	3.3
1	B	471[A]	ARG	3.3
1	D	438	ASP	3.3
1	D	273	THR	3.3
1	B	653	VAL	3.3
1	C	69	LEU	3.3
1	D	493	VAL	3.3
1	C	207	VAL	3.2
1	A	551	CYS	3.2
1	D	310	ARG	3.2
1	D	327	ILE	3.2
1	A	137	LEU	3.2
1	C	282	ALA	3.2
1	C	489	LYS	3.2
1	D	69	LEU	3.2
1	D	178	PRO	3.1
1	C	340	LEU	3.1
1	C	179	ASN	3.1
1	B	740	HIS	3.1
1	A	207	VAL	3.1
1	A	711	VAL	3.1
1	C	82	GLU	3.1
1	D	393	ASP	3.1
1	B	654	ALA	3.0
1	A	69	LEU	3.0
1	C	491	LEU	3.0
1	D	96	ASP	3.0
1	D	444	CYS	3.0
1	C	80	ASN	3.0
1	D	337	TRP	3.0
1	D	328	CYS	3.0
1	D	342	ALA	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	392	LYS	3.0
1	C	506	ASN	3.0
1	C	336	ARG	3.0
1	D	413	ASP	3.0
1	C	114	ILE	3.0
1	B	628	GLY	3.0
1	C	94	THR	3.0
1	C	81	ALA	2.9
1	A	547	TYR	2.9
1	B	630	SER	2.9
1	D	95	PHE	2.9
1	B	546	VAL	2.9
1	B	547	TYR	2.9
1	C	105	TYR	2.9
1	D	334	SER	2.9
1	C	283	THR	2.9
1	B	733	MET	2.9
1	C	142	LEU	2.9
1	C	335	GLY	2.9
1	C	75	ASN	2.9
1	D	489	LYS	2.9
1	D	412	SER	2.9
1	D	441	LYS	2.9
1	C	490	GLY	2.9
1	C	79	PHE	2.9
1	D	173	TYR	2.9
1	D	287	ILE	2.9
1	D	742	ILE	2.9
1	D	400	GLY	2.8
1	D	394	CYS	2.8
1	B	90	LEU	2.8
1	D	431	LEU	2.8
1	D	435	GLN	2.8
1	D	114	ILE	2.8
1	C	332	GLU	2.8
1	D	629	TRP	2.8
1	B	142	LEU	2.8
1	D	344	GLN	2.8
1	B	140	ARG	2.8
1	B	631	TYR	2.8
1	D	179	ASN	2.8
1	C	102	ILE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	703	ILE	2.8
1	D	434	ILE	2.7
1	B	666	TYR	2.7
1	C	70	TYR	2.7
1	C	210	ALA	2.7
1	D	72	GLN	2.7
1	D	486	VAL	2.7
1	B	357	PHE	2.7
1	D	336	ARG	2.7
1	B	138	ASN	2.7
1	D	269	PHE	2.7
1	A	105	TYR	2.7
1	B	521	GLU	2.7
1	B	711	VAL	2.7
1	C	54	ARG	2.7
1	C	99	GLY	2.7
1	C	388	GLN	2.7
1	C	653	VAL	2.7
1	D	384	ILE	2.7
1	D	390	ASP	2.7
1	B	87	SER	2.6
1	C	333	SER	2.6
1	D	61	ARG	2.6
1	A	145	GLU	2.6
1	C	91	GLU	2.6
1	B	71	LYS	2.6
1	D	343	ARG	2.6
1	B	703	ILE	2.6
1	C	140	ARG	2.6
1	D	285	ILE	2.6
1	D	487	ASN	2.6
1	D	521	GLU	2.6
1	C	711	VAL	2.6
1	D	223	LEU	2.6
1	D	388	GLN	2.6
1	C	145	GLU	2.6
1	D	378	GLU	2.6
1	D	409	ALA	2.6
1	D	462	SER	2.5
1	D	488	ASP	2.5
1	D	653	VAL	2.5
1	C	181	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	2.5
1	D	443	THR	2.5
1	C	392	LYS	2.5
1	D	63	ILE	2.5
1	D	766	PRO	2.5
1	D	85	ASN	2.5
1	A	552	SER	2.5
1	C	209	SER	2.5
1	A	740	HIS	2.5
1	B	705	GLY	2.5
1	C	278	SER	2.5
1	D	630	SER	2.5
1	B	518	ILE	2.5
1	D	469	GLN	2.4
1	A	143	ILE	2.4
1	C	147	ARG	2.4
1	A	142	LEU	2.4
1	D	187	TRP	2.4
1	C	208	PHE	2.4
1	A	144	THR	2.4
1	A	666	TYR	2.4
1	C	118	TYR	2.4
1	C	132	TYR	2.4
1	A	148	ILE	2.4
1	D	160	VAL	2.4
1	D	734	TRP	2.4
1	B	99	GLY	2.4
1	D	86	SER	2.4
1	A	166	TYR	2.4
1	B	139	LYS	2.4
1	D	402	TRP	2.4
1	A	357	PHE	2.4
1	B	205	GLU	2.4
1	B	210	ALA	2.4
1	D	136	ASP	2.4
1	B	86	SER	2.4
1	C	537	SER	2.4
1	D	656	VAL	2.3
1	A	201	TRP	2.3
1	C	650	GLY	2.3
1	B	63	ILE	2.3
1	A	399	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	336	ARG	2.3
1	B	755	MET	2.3
1	B	505	GLN	2.3
1	C	651	ILE	2.3
1	A	208	PHE	2.3
1	D	477	LEU	2.3
1	A	274	ASP	2.3
1	A	210	ALA	2.3
1	D	422	TYR	2.3
1	B	84	GLY	2.3
1	C	505	GLN	2.3
1	A	71	LYS	2.2
1	B	328	CYS	2.2
1	B	442	VAL	2.2
1	C	41	LYS	2.2
1	C	139	LYS	2.2
1	D	399	LYS	2.2
1	C	504	LEU	2.2
1	D	530	LEU	2.2
1	B	76	ILE	2.2
1	A	54	ARG	2.2
1	B	141	GLN	2.2
1	C	276	LEU	2.2
1	D	164	LEU	2.2
1	A	630	SER	2.2
1	A	85	ASN	2.2
1	C	487	ASN	2.2
1	C	713	PHE	2.2
1	D	329	ASP	2.2
1	D	340	LEU	2.2
1	A	162	HIS	2.2
1	A	506	ASN	2.2
1	D	219	ASN	2.2
1	C	702	LEU	2.2
1	C	536	LYS	2.2
1	A	707	ALA	2.2
1	C	143	ILE	2.2
1	B	627	TRP	2.2
1	A	632	GLY	2.2
1	B	467	TYR	2.2
1	D	147	ARG	2.2
1	A	102	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	708	ASP	2.1
1	A	546	VAL	2.1
1	A	665	VAL	2.1
1	B	558	VAL	2.1
1	C	187	TRP	2.1
1	D	305	TRP	2.1
1	C	666	TYR	2.1
1	B	702	LEU	2.1
1	A	502	LYS	2.1
1	C	652	ALA	2.1
1	C	63	ILE	2.1
1	C	62	TRP	2.1
1	C	280	THR	2.1
1	A	181	PRO	2.1
1	D	459	VAL	2.1
1	A	670	TYR	2.1
1	A	77	LEU	2.1
1	C	701	LEU	2.1
1	D	506	ASN	2.1
1	B	651	ILE	2.1
1	D	535	ASP	2.1
1	C	734	TRP	2.1
1	D	216	TRP	2.1
1	A	209	SER	2.1
1	D	308	GLN	2.1
1	B	656	VAL	2.1
1	C	357	PHE	2.1
1	A	203	TYR	2.1
1	C	514	LEU	2.1
1	C	631	TYR	2.1
1	A	654	ALA	2.1
1	B	96	ASP	2.1
1	D	740	HIS	2.1
1	D	751	ILE	2.1
1	C	271	VAL	2.1
1	C	710	ASN	2.0
1	C	135	TYR	2.0
1	B	655	PRO	2.0
1	C	334	SER	2.0
1	D	144	THR	2.0
1	D	733	MET	2.0
1	C	630	SER	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	124	TRP	2.0
1	C	281	ASN	2.0
1	D	466	LYS	2.0
1	D	505	GLN	2.0
1	C	708	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	804	14/15	0.93	0.17	1.53	56,59,62,65	0
4	NAG	B	804	14/15	0.91	0.19	1.00	62,65,69,73	0
4	NAG	C	803	14/15	0.92	0.14	-0.27	60,63,66,70	0
4	NAG	D	802	14/15	0.93	0.12	-1.67	60,63,65,69	0
4	NAG	A	807	14/15	0.81	0.20	-	90,91,92,92	0
4	NAG	A	806	14/15	0.70	0.20	-	80,84,85,87	0
4	NAG	C	804	14/15	0.87	0.18	-	73,75,77,77	0
4	NAG	D	803	14/15	0.88	0.12	-	73,75,76,77	0
4	NAG	A	805	14/15	0.83	0.14	-	67,68,69,69	0
4	NAG	B	805	14/15	0.84	0.26	-	77,79,80,80	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	806	14/15	0.84	0.20	2.65	68,73,74,74	0
2	XIH	A	800	29/29	0.97	0.28	0.85	38,43,44,44	0
2	XIH	D	800	29/29	0.96	0.23	0.50	40,42,43,45	0
3	NAG	A	808	14/15	0.94	0.18	0.47	62,66,68,68	0
3	NAG	A	801	14/15	0.62	0.29	0.32	95,95,96,96	0
2	XIH	B	800	29/29	0.96	0.27	-0.04	35,39,40,41	0
2	XIH	C	800	29/29	0.97	0.23	-0.51	35,37,38,39	0
3	NAG	A	802	14/15	0.66	0.30	-	75,78,79,79	0
3	NAG	D	804	14/15	0.77	0.13	-	81,83,85,85	0
3	NAG	C	801	14/15	0.74	0.20	-	60,60,61,62	0
3	NAG	A	803	14/15	0.79	0.22	-	69,72,76,77	0
3	NAG	B	802	14/15	0.85	0.16	-	67,68,69,70	0
3	NAG	C	805	14/15	0.69	0.20	-	78,81,82,82	0
3	NAG	B	801	14/15	0.67	0.16	-	79,80,81,81	0
3	NAG	B	806	14/15	0.72	0.14	-	69,71,74,74	0
3	NAG	D	801	14/15	0.85	0.18	-	65,67,68,69	0
3	NAG	C	802	14/15	0.86	0.15	-	70,72,75,75	0
3	NAG	B	803	14/15	0.80	0.24	-	64,67,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.