



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 01:52 PM EDT

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 : unknown  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

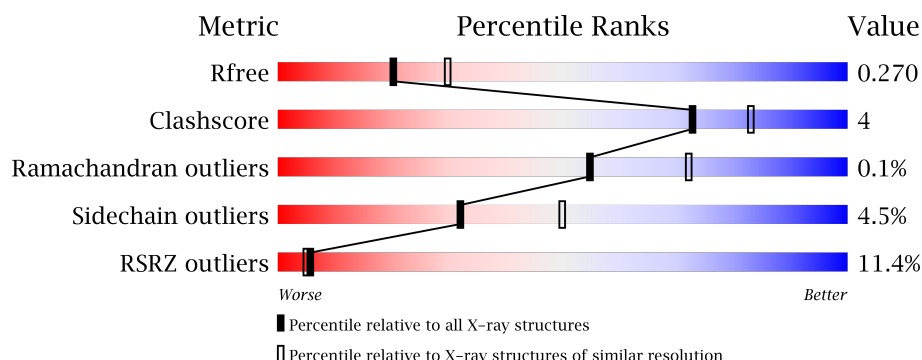
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	740	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	740	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	740	<div> <div>19%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	806	-	-	-	X
3	NAG	D	804	X	-	-	-

## 2 Entry composition

There are 4 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:

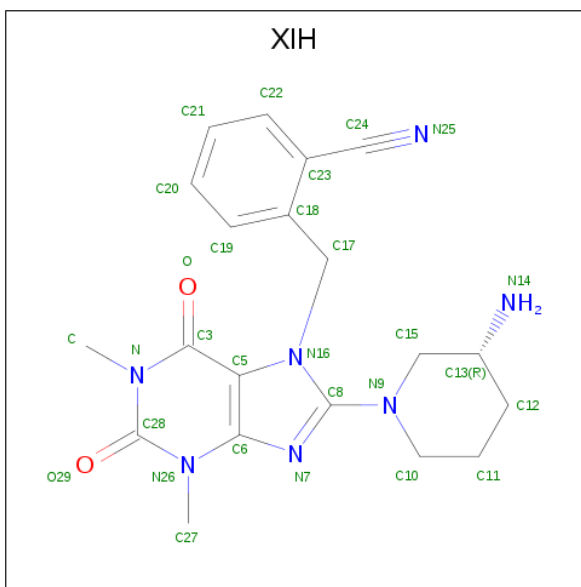
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487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

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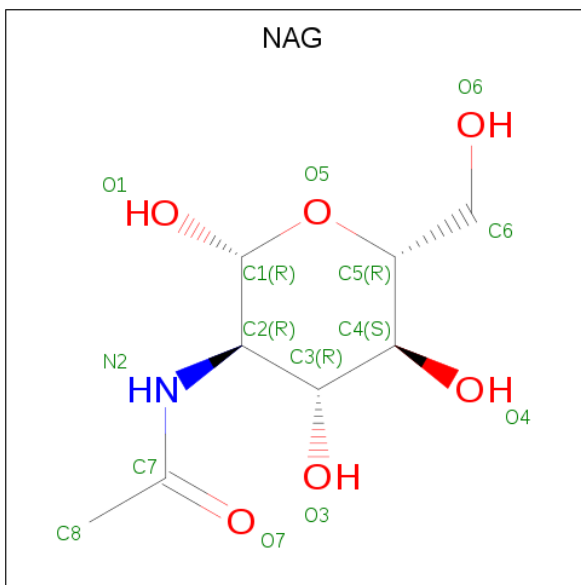
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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 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	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	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	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 water.

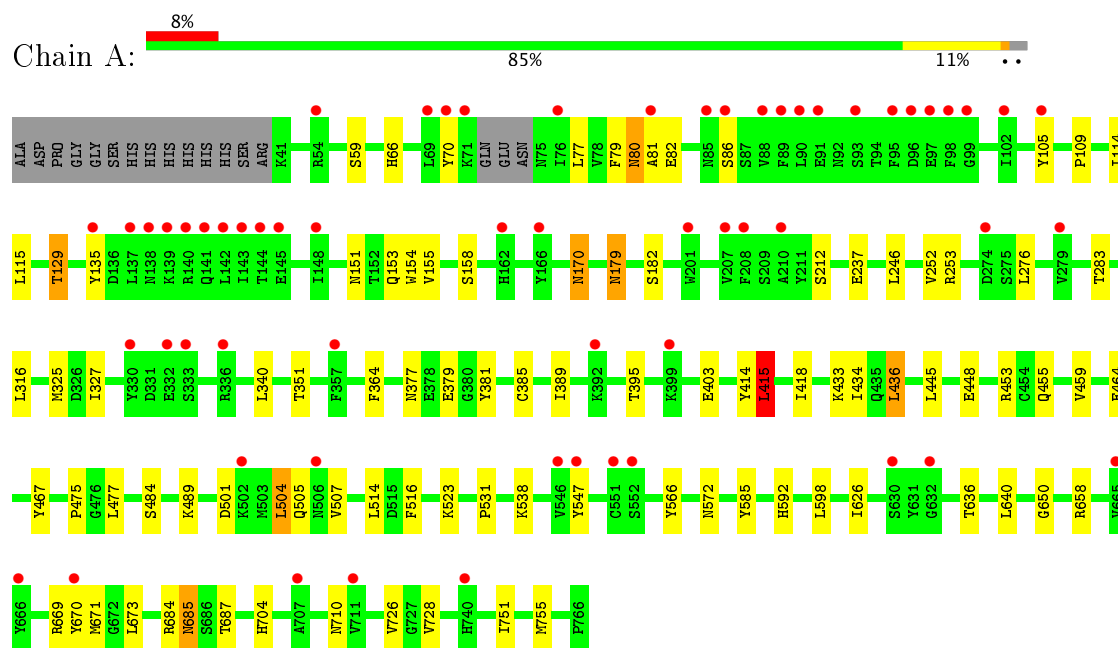
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	394	Total	O	0	0
			394	394		
4	B	370	Total	O	0	0
			370	370		
4	C	348	Total	O	0	0
			348	348		
4	D	215	Total	O	0	0
			215	215		



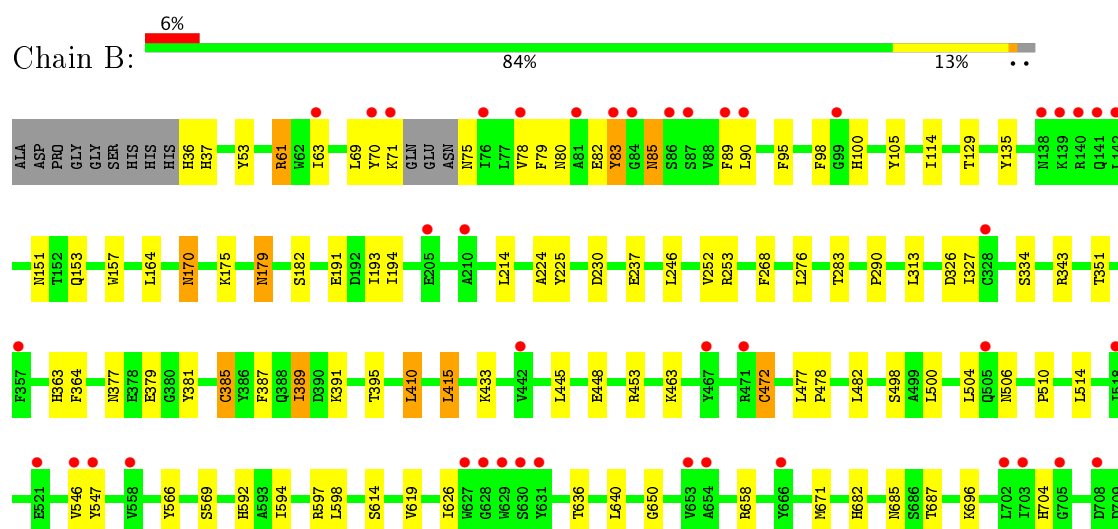
### 3 Residue-property plots [i](#)

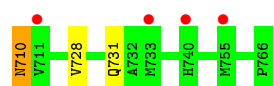
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Dipeptidyl peptidase 4

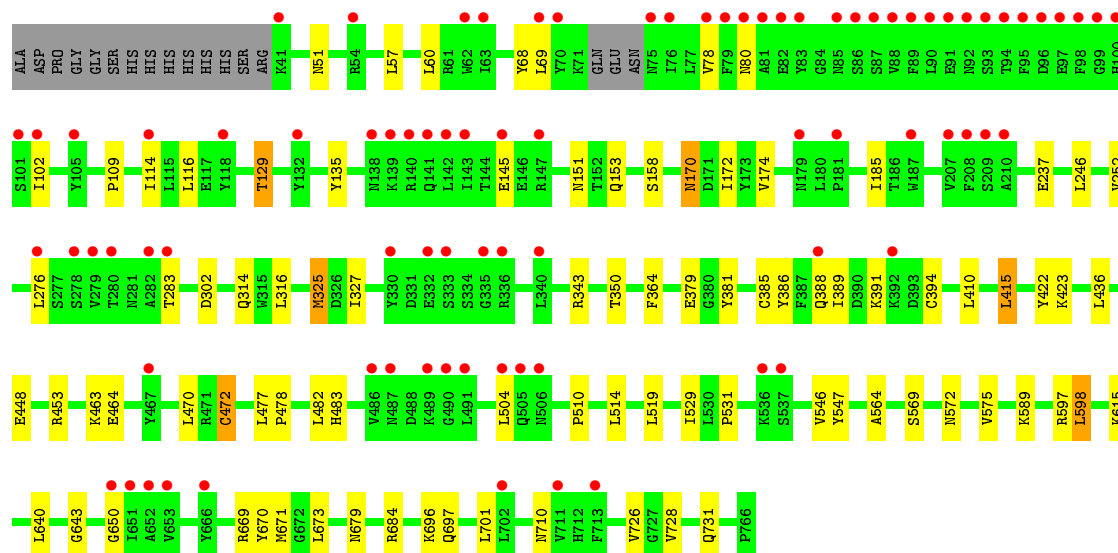
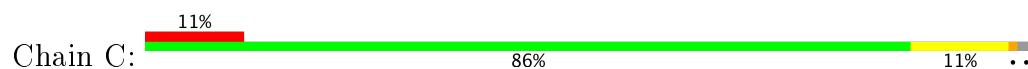


#### • Molecule 1: Dipeptidyl peptidase 4

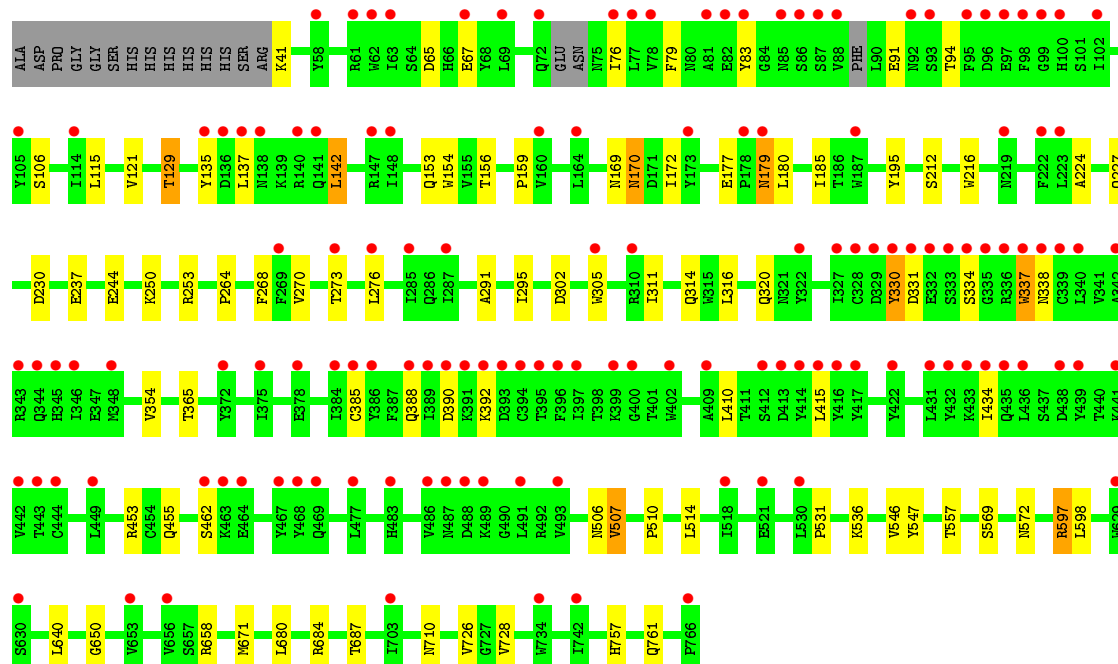
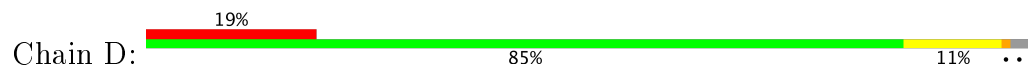




• Molecule 1: Dipeptidyl peptidase 4



• 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	Depositor
R, $R_{free}$	0.187 , 0.239 0.230 , 0.270	Depositor DCC
$R_{free}$ test set	7417 reflections (5.02%)	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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	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, 0.333 respectively for untwinned datasets, and 0.375, 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	112	0	102	0	0
3	B	84	0	77	0	0
3	C	84	0	77	0	0
3	D	56	0	51	0	0
4	A	394	0	0	2	0
4	B	370	0	0	1	0
4	C	348	0	0	1	0
4	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
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.23	0.73
1:B:731[B]:GLN:HG3	4: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:597:ARG:HH11	1:B:682:HIS:HB2	1.72	0.54
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.89	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
1:C:343:ARG:HD2	1:C:389:ILE:HG23	1.91	0.52
1:A:80:ASN:HD22	1:A:82:GLU:H	1.58	0.52
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.92	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ALA:O	1:D:295:ILE:HG23	2.09	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:A:179:ASN:N	1:A:179:ASN:HD22	2.07	0.51
1:B:377:ASN:OD1	1:B:379:GLU:HG2	2.11	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:114:ILE:CG2	1:A:135:TYR:HB3	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.92	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	4: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:364:PHE:HE2	1:A:389:ILE:HD11	1.79	0.48
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.95	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	4:D:1339:HOH:O	1.97	0.47
1:D:91:GLU:HB3	1:D:94:THR:OG1	2.15	0.47
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:129:THR:HG21	1:A:151:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.97	0.47
1:C:129:THR:HG23	1:C:151:ASN:HA	1.96	0.47
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.50	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	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	4:C:1004:HOH:O	2.15	0.46
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.98	0.46
1:A:467:TYR:HD2	1:A:484:SER:HA	1.81	0.46
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.98	0.46
1:D:179:ASN:ND2	1:D:179:ASN:H	2.11	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:B:433:LYS:HD2	1:B:445:LEU:HD21	1.98	0.46
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.46
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.44	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:B:626:ILE:HG23	1:B:636:THR:HG23	1.99	0.44
1:C:302:ASP:HB3	1:C:314:GLN:HB2	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
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.99	0.43
1:D:76:ILE:H	1:D:91:GLU:HA	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:626:ILE:HG23	1:A:636:THR:HG23	1.99	0.43
1:A:685:ASN:ND2	4:A:981:HOH:O	2.51	0.43
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.53	0.43
1:A:415:LEU:HB2	1:A:436:LEU:HD11	2.00	0.43
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.99	0.43
1:D:597:ARG:HA	1:D:597:ARG:HD3	1.84	0.43
1:B:598:LEU:O	1:B:682:HIS:NE2	2.48	0.43
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.43
1:B:598:LEU:HB2	1:B:671:MET:SD	2.59	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:A:109:PRO:HG2	1:A:158:SER:O	2.18	0.42
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.49	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:A:504:LEU:HA	1:A:507:VAL:HG12	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.03	0.41
1:B:191:GLU:O	1:B:193:ILE:HD12	2.20	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:B:98:PHE:CE1	1:B:100:HIS:HB2	2.55	0.41
1:D:169:ASN:O	1:D:170:ASN:HB2	2.21	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
1:B:82:GLU:HB2	1:B:83:TYR:CD1	2.56	0.40
1:C:109:PRO:HG2	1:C:158:SER:O	2.21	0.40
1:C:386:TYR:O	1:C:394:CYS:HB2	2.21	0.40
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:510:PRO:HD3	1:C:569:SER:HB2	2.04	0.40
1:C:60:LEU:HB2	1:C:68:TYR:CD1	2.56	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%)	55	72
1	C	720/740 (97%)	692 (96%)	28 (4%)	0	100	100
1	D	717/740 (97%)	687 (96%)	29 (4%)	1 (0%)	55	72
All	All	2886/2960 (98%)	2771 (96%)	113 (4%)	2 (0%)	55	72

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/662 (98%)	623 (96%)	28 (4%)	33	52
1	B	654/662 (99%)	620 (95%)	34 (5%)	27	43
1	C	649/662 (98%)	616 (95%)	33 (5%)	28	44
1	D	648/662 (98%)	625 (96%)	23 (4%)	41	61
All	All	2602/2648 (98%)	2484 (96%)	118 (4%)	32	50

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
1	A	673	LEU
1	A	685	ASN
1	A	704	HIS
1	A	710	ASN

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Mol	Chain	Res	Type
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
1	C	145	GLU
1	C	170	ASN
1	C	246	LEU
1	C	276	LEU

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Mol	Chain	Res	Type
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
1	D	453	ARG
1	D	506	ASN
1	D	507	VAL
1	D	514	LEU

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Mol	Chain	Res	Type
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
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	572	ASN

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Mol	Chain	Res	Type
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 [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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

28 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	-	24,32,32	2.12	3 (12%)	29,47,47	2.07	8 (27%)
3	NAG	A	801	1	14,14,15	0.51	0	15,19,21	0.84	1 (6%)
3	NAG	A	802	1	14,14,15	0.51	0	15,19,21	0.90	1 (6%)
3	NAG	A	803	1	14,14,15	0.52	0	15,19,21	0.92	0
3	NAG	A	804	1,3	14,14,15	0.65	0	15,19,21	1.23	1 (6%)
3	NAG	A	805	3	14,14,15	0.44	0	15,19,21	1.09	1 (6%)
3	NAG	A	806	1,3	14,14,15	0.49	0	15,19,21	1.30	2 (13%)
3	NAG	A	807	3	14,14,15	0.51	0	15,19,21	0.78	0
3	NAG	A	808	1	14,14,15	0.54	0	15,19,21	1.20	1 (6%)
2	XIH	B	800	-	24,32,32	2.12	3 (12%)	29,47,47	2.06	9 (31%)
3	NAG	B	801	1	14,14,15	0.69	0	15,19,21	1.37	2 (13%)
3	NAG	B	802	1	14,14,15	0.52	0	15,19,21	1.54	1 (6%)
3	NAG	B	803	1	14,14,15	0.60	0	15,19,21	0.99	1 (6%)
3	NAG	B	804	1,3	14,14,15	0.58	0	15,19,21	0.98	0
3	NAG	B	805	3	14,14,15	0.51	0	15,19,21	1.47	2 (13%)
3	NAG	B	806	1	14,14,15	0.49	0	15,19,21	1.46	3 (20%)
2	XIH	C	800	-	24,32,32	2.34	4 (16%)	29,47,47	2.02	10 (34%)
3	NAG	C	801	1	14,14,15	0.61	0	15,19,21	1.06	1 (6%)
3	NAG	C	802	1	14,14,15	0.60	0	15,19,21	1.02	1 (6%)
3	NAG	C	803	1,3	14,14,15	0.60	0	15,19,21	1.05	1 (6%)
3	NAG	C	804	3	14,14,15	0.49	0	15,19,21	0.81	1 (6%)
3	NAG	C	805	1	14,14,15	0.61	0	15,19,21	1.09	1 (6%)
3	NAG	C	806	1	14,14,15	0.52	0	15,19,21	0.96	0
2	XIH	D	800	-	24,32,32	2.32	3 (12%)	29,47,47	1.83	6 (20%)
3	NAG	D	801	1	14,14,15	0.55	0	15,19,21	1.02	2 (13%)
3	NAG	D	802	1,3	14,14,15	0.48	0	15,19,21	1.11	2 (13%)
3	NAG	D	803	3	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
3	NAG	D	804	1	14,14,15	0.61	0	15,19,21	1.49	3 (20%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	807	3	-	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	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	805	3	-	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	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	804	3	-	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	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	3	-	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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	XIH	C23-C24	-9.35	1.29	1.44
2	D	800	XIH	C23-C24	-9.32	1.29	1.44
2	B	800	XIH	C23-C24	-8.74	1.30	1.44
2	A	800	XIH	C23-C24	-8.46	1.30	1.44
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	3.75	1.47	1.41
2	C	800	XIH	C3-C5	4.36	1.48	1.41
2	A	800	XIH	C3-C5	4.63	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	XIH	C3-C5	4.86	1.49	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	XIH	C3-C5-C6	-3.80	117.30	119.92
3	A	804	NAG	O5-C1-C2	-3.39	106.75	111.47
2	C	800	XIH	C11-C12-C13	-3.19	107.73	111.97
3	A	806	NAG	O5-C1-C2	-2.90	107.43	111.47
2	D	800	XIH	C3-C5-C6	-2.85	117.96	119.92
2	C	800	XIH	C17-C18-C19	-2.76	114.99	121.17
2	D	800	XIH	C10-N9-C8	-2.75	115.95	122.07
2	C	800	XIH	C3-C5-C6	-2.72	118.05	119.92
2	A	800	XIH	C17-C18-C19	-2.60	115.36	121.17
2	B	800	XIH	C10-N9-C8	-2.51	116.48	122.07
3	D	802	NAG	O5-C1-C2	-2.45	108.06	111.47
2	C	800	XIH	C10-N9-C8	-2.36	116.81	122.07
3	B	806	NAG	C4-C3-C2	-2.28	107.68	111.02
2	B	800	XIH	C3-C5-C6	-2.27	118.36	119.92
2	B	800	XIH	C17-C18-C19	-2.26	116.12	121.17
2	A	800	XIH	C10-N9-C8	-2.10	117.38	122.07
3	C	804	NAG	O5-C1-C2	-2.04	108.64	111.47
3	B	806	NAG	C3-C4-C5	-2.03	106.63	110.22
3	D	801	NAG	C1-O5-C5	2.03	114.96	112.17
3	D	802	NAG	C1-O5-C5	2.06	115.01	112.17
2	D	800	XIH	C27-N26-C6	2.08	121.27	118.31
3	D	801	NAG	C4-C3-C2	2.08	114.07	111.02
2	B	800	XIH	C11-C10-N9	2.16	115.35	111.09
2	C	800	XIH	C12-C11-C10	2.19	113.84	110.96
3	B	803	NAG	C1-O5-C5	2.21	115.21	112.17
2	A	800	XIH	C19-C18-C23	2.22	120.02	117.53
2	D	800	XIH	C17-C18-C23	2.30	123.55	120.45
3	A	801	NAG	C1-O5-C5	2.34	115.39	112.17
3	C	802	NAG	C4-C3-C2	2.34	114.44	111.02
2	B	800	XIH	C27-N26-C6	2.34	121.65	118.31
2	C	800	XIH	C18-C23-C24	2.34	122.56	120.24
3	C	803	NAG	C4-C3-C2	2.35	114.46	111.02
3	B	805	NAG	O5-C1-C2	2.37	114.78	111.47
3	B	801	NAG	O5-C1-C2	2.49	114.94	111.47
2	C	800	XIH	C19-C18-C23	2.53	120.36	117.53
3	D	804	NAG	O5-C1-C2	2.57	115.05	111.47
3	D	803	NAG	C1-O5-C5	2.62	115.78	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	NAG	C1-O5-C5	2.65	115.82	112.17
3	A	806	NAG	C1-O5-C5	2.70	115.89	112.17
3	D	804	NAG	C1-O5-C5	2.88	116.13	112.17
3	C	805	NAG	C1-O5-C5	2.89	116.15	112.17
3	A	802	NAG	C1-O5-C5	3.00	116.31	112.17
2	C	800	XIH	C17-C18-C23	3.07	124.59	120.45
2	A	800	XIH	C17-C18-C23	3.08	124.61	120.45
3	D	804	NAG	C4-C3-C2	3.09	115.55	111.02
2	B	800	XIH	C17-C18-C23	3.17	124.72	120.45
2	A	800	XIH	C18-C23-C24	3.21	123.41	120.24
3	A	805	NAG	C1-O5-C5	3.31	116.73	112.17
2	B	800	XIH	C18-C23-C24	3.32	123.52	120.24
3	A	808	NAG	C1-O5-C5	3.37	116.81	112.17
3	B	801	NAG	C4-C3-C2	3.38	115.97	111.02
2	A	800	XIH	C18-C17-N16	3.90	119.78	113.31
2	B	800	XIH	C18-C17-N16	3.95	119.87	113.31
3	B	806	NAG	C1-O5-C5	3.97	117.64	112.17
2	D	800	XIH	C18-C17-N16	4.03	120.00	113.31
2	C	800	XIH	C18-C17-N16	4.44	120.68	113.31
3	B	805	NAG	C1-O5-C5	4.62	118.54	112.17
3	B	802	NAG	C1-O5-C5	4.87	118.88	112.17
2	C	800	XIH	C10-N9-C15	5.40	123.47	113.14
2	D	800	XIH	C10-N9-C15	5.85	124.33	113.14
2	A	800	XIH	C10-N9-C15	5.91	124.45	113.14
2	B	800	XIH	C10-N9-C15	6.01	124.64	113.14

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.64	60 (8%) 12 11	39, 48, 74, 104	0
1	B	728/740 (98%)	0.49	47 (6%) 20 18	36, 49, 72, 93	0
1	C	723/740 (97%)	0.73	84 (11%) 5 5	39, 49, 73, 93	0
1	D	723/740 (97%)	1.07	138 (19%) 1 1	38, 54, 82, 118	0
All	All	2897/2960 (97%)	0.73	329 (11%) 6 5	36, 50, 76, 118	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	7.6
1	A	81	ALA	7.4
1	D	77	LEU	7.2
1	D	92	ASN	7.1
1	C	279	VAL	6.9
1	B	81	ALA	6.9
1	D	322	TYR	6.5
1	C	89	PHE	6.3
1	D	467	TYR	5.8
1	D	415	LEU	5.7
1	A	86	SER	5.6
1	C	83	TYR	5.5
1	D	333	SER	5.5
1	D	416	TYR	5.4
1	A	95	PHE	5.4
1	C	93	SER	5.3
1	D	372	TYR	5.3
1	A	135	TYR	5.2
1	D	97	GLU	5.2
1	D	396	PHE	5.1
1	D	397	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	5.1
1	D	135	TYR	5.1
1	C	76	ILE	5.1
1	D	81	ALA	5.0
1	D	386	TYR	5.0
1	B	78	VAL	4.9
1	D	464	GLU	4.9
1	D	98	PHE	4.9
1	D	148	ILE	4.8
1	D	93	SER	4.8
1	D	138	ASN	4.8
1	D	141	GLN	4.7
1	C	97	GLU	4.7
1	D	391	LYS	4.7
1	A	90	LEU	4.7
1	C	90	LEU	4.7
1	D	468	TYR	4.6
1	D	62	TRP	4.6
1	C	87	SER	4.6
1	D	335	GLY	4.5
1	D	392	LYS	4.5
1	D	78	VAL	4.5
1	D	442	VAL	4.5
1	C	330	TYR	4.4
1	A	140	ARG	4.4
1	A	93	SER	4.4
1	C	96	ASP	4.4
1	C	95	PHE	4.3
1	A	141	GLN	4.3
1	D	140	ARG	4.3
1	C	98	PHE	4.3
1	D	330	TYR	4.2
1	D	414	TYR	4.2
1	A	332	GLU	4.2
1	C	138	ASN	4.1
1	D	389	ILE	4.1
1	B	70	TYR	4.1
1	D	105	TYR	4.1
1	A	88	VAL	4.0
1	D	332	GLU	4.0
1	D	395	THR	4.0
1	C	86	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	137	LEU	3.9
1	D	439	TYR	3.9
1	D	491	LEU	3.9
1	D	339	CYS	3.9
1	C	467	TYR	3.8
1	D	222	PHE	3.8
1	D	83	TYR	3.8
1	C	78	VAL	3.8
1	D	88	VAL	3.8
1	D	417	TYR	3.7
1	D	102	ILE	3.7
1	D	449	LEU	3.7
1	D	375	ILE	3.7
1	D	338	ASN	3.7
1	A	76	ILE	3.6
1	D	82	GLU	3.6
1	B	89	PHE	3.6
1	C	486	VAL	3.6
1	A	97	GLU	3.6
1	D	348	MET	3.6
1	D	483	HIS	3.6
1	A	139	LYS	3.6
1	C	85	ASN	3.5
1	A	70	TYR	3.5
1	C	141	GLN	3.5
1	A	91	GLU	3.4
1	A	96	ASP	3.4
1	A	98	PHE	3.4
1	D	432	TYR	3.4
1	A	99	GLY	3.4
1	C	101	SER	3.4
1	A	138	ASN	3.4
1	D	463	LYS	3.4
1	D	433	LYS	3.4
1	D	346	ILE	3.3
1	D	331	ASP	3.3
1	D	100	HIS	3.3
1	D	67	GLU	3.3
1	D	276	LEU	3.3
1	D	345	HIS	3.3
1	B	83	TYR	3.3
1	C	92	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	89	PHE	3.3
1	D	87	SER	3.2
1	D	436	LEU	3.2
1	D	76	ILE	3.2
1	B	471[A]	ARG	3.2
1	D	58	TYR	3.2
1	D	518	ILE	3.2
1	A	333	SER	3.2
1	D	438	ASP	3.2
1	C	100	HIS	3.2
1	A	279	VAL	3.2
1	B	629	TRP	3.2
1	D	385	CYS	3.2
1	D	310	ARG	3.1
1	C	69	LEU	3.1
1	D	273	THR	3.1
1	C	489	LYS	3.1
1	B	653	VAL	3.1
1	D	493	VAL	3.1
1	C	207	VAL	3.1
1	A	137	LEU	3.1
1	D	327	ILE	3.1
1	C	282	ALA	3.1
1	D	69	LEU	3.0
1	A	551	CYS	3.0
1	D	178	PRO	3.0
1	C	82	GLU	3.0
1	C	340	LEU	3.0
1	C	179	ASN	3.0
1	B	740	HIS	3.0
1	D	393	ASP	2.9
1	A	207	VAL	2.9
1	A	711	VAL	2.9
1	A	392	LYS	2.9
1	D	96	ASP	2.9
1	A	69	LEU	2.9
1	C	491	LEU	2.9
1	B	654	ALA	2.9
1	C	336	ARG	2.9
1	C	80	ASN	2.9
1	D	337	TRP	2.9
1	C	506	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	342	ALA	2.9
1	D	444	CYS	2.9
1	D	413	ASP	2.9
1	D	328	CYS	2.8
1	A	547	TYR	2.8
1	C	114	ILE	2.8
1	B	628	GLY	2.8
1	B	547	TYR	2.8
1	B	630	SER	2.8
1	C	94	THR	2.8
1	C	105	TYR	2.8
1	D	95	PHE	2.8
1	D	489	LYS	2.8
1	C	81	ALA	2.8
1	D	334	SER	2.8
1	D	441	LYS	2.8
1	B	733	MET	2.8
1	B	546	VAL	2.8
1	C	75	ASN	2.8
1	C	142	LEU	2.8
1	C	335	GLY	2.8
1	C	283	THR	2.8
1	D	173	TYR	2.8
1	D	412	SER	2.7
1	D	435	GLN	2.7
1	C	490	GLY	2.7
1	C	79	PHE	2.7
1	C	332	GLU	2.7
1	D	287	ILE	2.7
1	D	742	ILE	2.7
1	D	400	GLY	2.7
1	B	90	LEU	2.7
1	D	431	LEU	2.7
1	B	140	ARG	2.7
1	D	344	GLN	2.7
1	D	629	TRP	2.7
1	D	114	ILE	2.7
1	B	631	TYR	2.7
1	B	142	LEU	2.7
1	D	394	CYS	2.7
1	D	179	ASN	2.7
1	D	72	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	666	TYR	2.6
1	C	70	TYR	2.6
1	D	336	ARG	2.6
1	C	102	ILE	2.6
1	D	703	ILE	2.6
1	C	54	ARG	2.6
1	C	210	ALA	2.6
1	D	434	ILE	2.6
1	B	521	GLU	2.6
1	A	105	TYR	2.6
1	B	138	ASN	2.6
1	B	357	PHE	2.6
1	C	388	GLN	2.6
1	D	269	PHE	2.6
1	D	486	VAL	2.6
1	D	61	ARG	2.6
1	C	99	GLY	2.6
1	B	71	LYS	2.6
1	B	711	VAL	2.5
1	D	390	ASP	2.5
1	A	145	GLU	2.5
1	C	91	GLU	2.5
1	D	343	ARG	2.5
1	B	87	SER	2.5
1	C	333	SER	2.5
1	D	384	ILE	2.5
1	C	653	VAL	2.5
1	C	140	ARG	2.5
1	D	521	GLU	2.5
1	D	388	GLN	2.5
1	B	703	ILE	2.5
1	D	487	ASN	2.5
1	C	145	GLU	2.5
1	D	378	GLU	2.5
1	D	285	ILE	2.5
1	D	223	LEU	2.5
1	C	392	LYS	2.4
1	D	488	ASP	2.4
1	D	462	SER	2.4
1	C	711	VAL	2.4
1	D	409	ALA	2.4
1	A	330	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	181	PRO	2.4
1	D	85	ASN	2.4
1	D	766	PRO	2.4
1	D	443	THR	2.4
1	D	653	VAL	2.4
1	A	552	SER	2.4
1	C	209	SER	2.4
1	D	63	ILE	2.4
1	A	740	HIS	2.4
1	C	278	SER	2.4
1	D	630	SER	2.4
1	B	705	GLY	2.4
1	D	469	GLN	2.4
1	C	147	ARG	2.3
1	B	518	ILE	2.3
1	B	139	LYS	2.3
1	A	143	ILE	2.3
1	A	142	LEU	2.3
1	A	666	TYR	2.3
1	C	118	TYR	2.3
1	C	132	TYR	2.3
1	D	187	TRP	2.3
1	C	208	PHE	2.3
1	B	205	GLU	2.3
1	A	144	THR	2.3
1	A	166	TYR	2.3
1	D	86	SER	2.3
1	B	99	GLY	2.3
1	D	734	TRP	2.3
1	A	148	ILE	2.3
1	A	357	PHE	2.3
1	D	160	VAL	2.3
1	D	402	TRP	2.3
1	D	136	ASP	2.3
1	B	86	SER	2.3
1	B	210	ALA	2.3
1	C	537	SER	2.3
1	A	399	LYS	2.2
1	A	336	ARG	2.2
1	B	505	GLN	2.2
1	A	201	TRP	2.2
1	C	650	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	755	MET	2.2
1	D	656	VAL	2.2
1	B	63	ILE	2.2
1	C	505	GLN	2.2
1	D	422	TYR	2.2
1	A	208	PHE	2.2
1	A	274	ASP	2.2
1	C	651	ILE	2.2
1	A	71	LYS	2.2
1	C	41	LYS	2.2
1	C	139	LYS	2.2
1	D	399	LYS	2.2
1	D	477	LEU	2.2
1	B	84	GLY	2.2
1	A	210	ALA	2.2
1	A	54	ARG	2.1
1	B	141	GLN	2.1
1	C	504	LEU	2.1
1	D	530	LEU	2.1
1	B	442	VAL	2.1
1	C	536	LYS	2.1
1	A	85	ASN	2.1
1	A	630	SER	2.1
1	B	76	ILE	2.1
1	C	487	ASN	2.1
1	C	276	LEU	2.1
1	D	164	LEU	2.1
1	B	328	CYS	2.1
1	D	329	ASP	2.1
1	C	713	PHE	2.1
1	D	147	ARG	2.1
1	A	506	ASN	2.1
1	D	219	ASN	2.1
1	D	340	LEU	2.1
1	A	162	HIS	2.1
1	A	502	LYS	2.1
1	B	467	TYR	2.1
1	C	702	LEU	2.1
1	A	707	ALA	2.1
1	A	632	GLY	2.1
1	B	627	TRP	2.1
1	C	666	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	708	ASP	2.0
1	C	143	ILE	2.0
1	C	187	TRP	2.0
1	D	305	TRP	2.0
1	A	102	ILE	2.0
1	B	702	LEU	2.0
1	C	652	ALA	2.0
1	A	546	VAL	2.0
1	A	665	VAL	2.0
1	B	558	VAL	2.0
1	A	670	TYR	2.0
1	C	62	TRP	2.0
1	C	63	ILE	2.0
1	C	280	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	NAG	C	806	14/15	0.84	0.20	2.65	68,73,74,74	0
3	NAG	A	804	14/15	0.93	0.17	1.53	56,59,62,65	0
3	NAG	B	804	14/15	0.91	0.19	1.00	62,65,69,73	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XIH	B	800	29/29	0.96	0.27	-0.04	35,39,40,41	0
3	NAG	C	803	14/15	0.92	0.14	-0.27	60,63,66,70	0
2	XIH	C	800	29/29	0.97	0.23	-0.51	35,37,38,39	0
3	NAG	D	802	14/15	0.93	0.12	-1.67	60,63,65,69	0
3	NAG	A	807	14/15	0.81	0.20	-	90,91,92,92	0
3	NAG	A	806	14/15	0.70	0.20	-	80,84,85,87	0
3	NAG	A	802	14/15	0.66	0.30	-	75,78,79,79	0
3	NAG	A	805	14/15	0.83	0.14	-	67,68,69,69	0
3	NAG	D	801	14/15	0.85	0.18	-	65,67,68,69	0
3	NAG	D	804	14/15	0.77	0.13	-	81,83,85,85	0
3	NAG	B	806	14/15	0.72	0.14	-	69,71,74,74	0
3	NAG	D	803	14/15	0.88	0.12	-	73,75,76,77	0
3	NAG	C	802	14/15	0.86	0.15	-	70,72,75,75	0
3	NAG	B	801	14/15	0.67	0.16	-	79,80,81,81	0
3	NAG	B	805	14/15	0.84	0.26	-	77,79,80,80	0
3	NAG	B	802	14/15	0.85	0.16	-	67,68,69,70	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	C	804	14/15	0.87	0.18	-	73,75,77,77	0
3	NAG	B	803	14/15	0.80	0.24	-	64,67,70,71	0
3	NAG	C	805	14/15	0.69	0.20	-	78,81,82,82	0

## 6.5 Other polymers

There are no such residues in this entry.