



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:48 pm 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

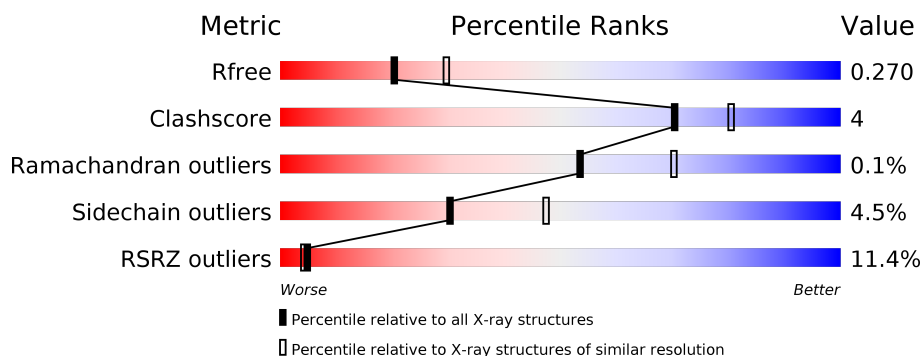
1 Overall quality at a glance ⓘ

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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (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 ≥ 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>85%</div> <div>11%</div> <div>..</div> </div>
1	B	740	<div> <div>6%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	740	<div> <div>11%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	D	740	<div> <div>19%</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	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:

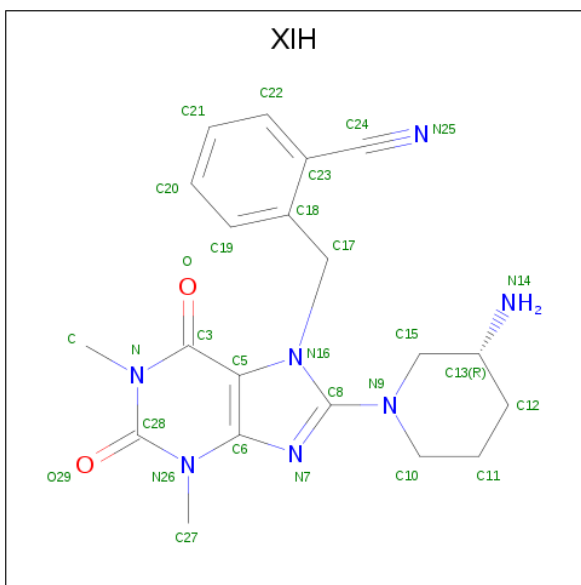
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
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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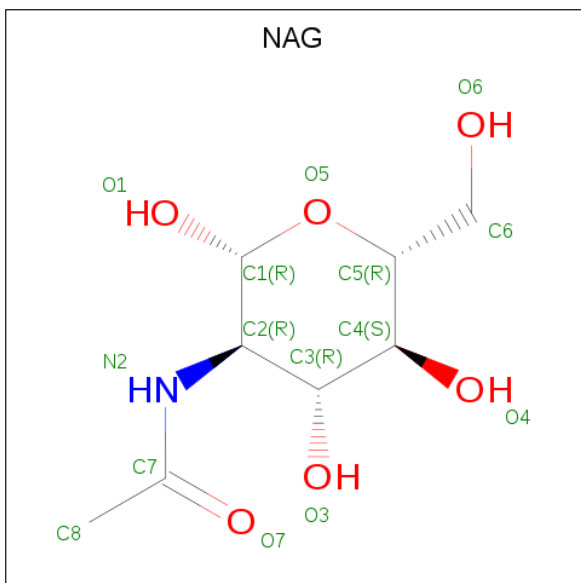
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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: C₂₀H₂₃N₇O₂).



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		

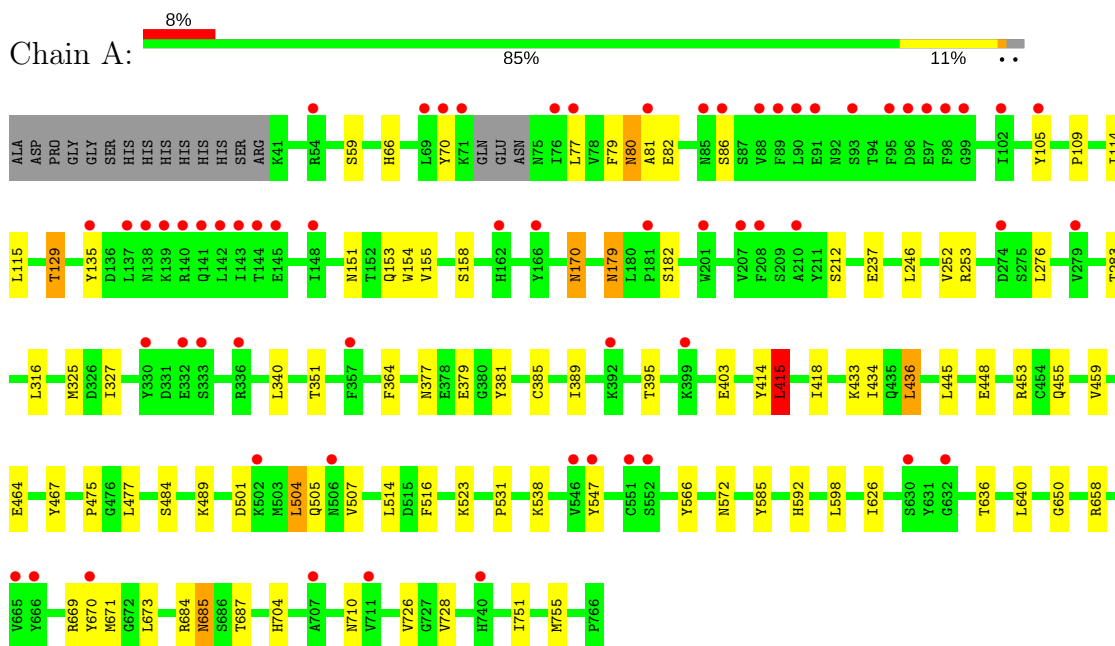
- Molecule 4 is water.

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		

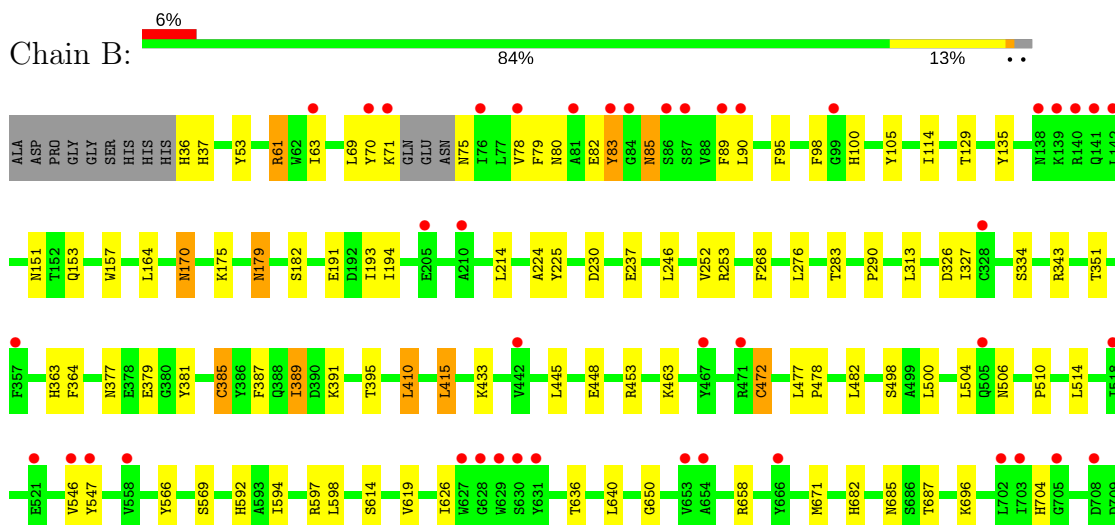
3 Residue-property plots [i](#)

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

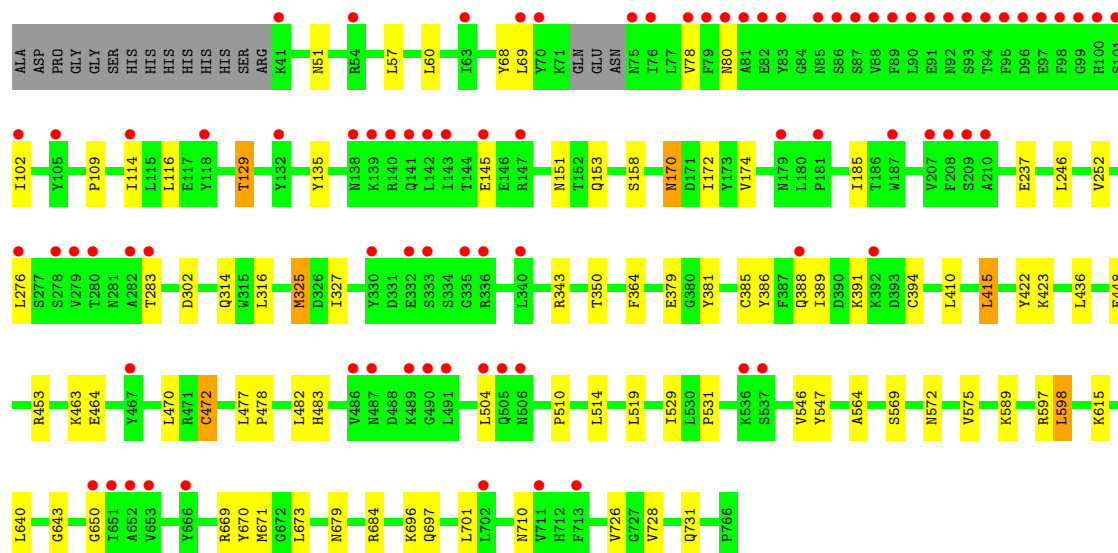
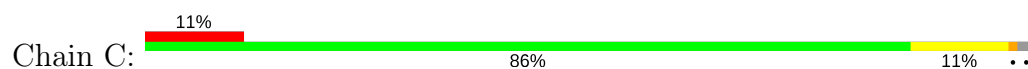


• Molecule 1: Dipeptidyl peptidase 4

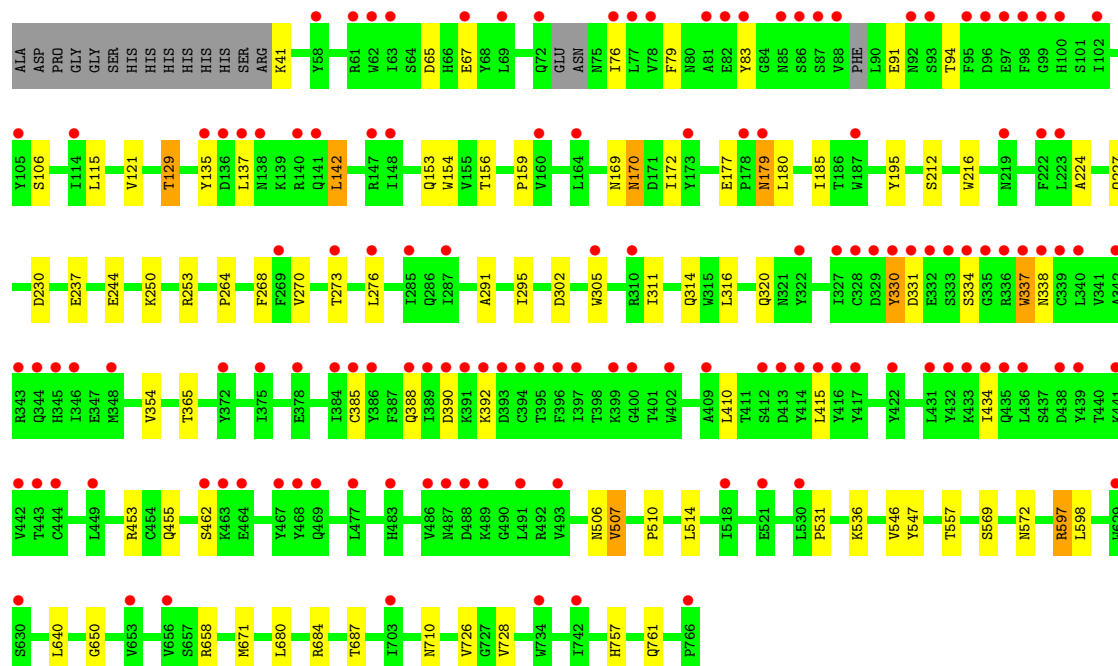
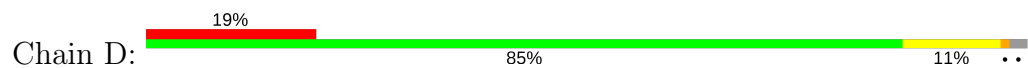




● Molecule 1: Dipeptidyl peptidase 4



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.239 0.231 , 0.270	Depositor DCC
R_{free} test set	7412 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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: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: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%)	53	70
1	C	720/740 (97%)	692 (96%)	28 (4%)	0	100	100
1	D	717/740 (97%)	687 (96%)	29 (4%)	1 (0%)	53	70
All	All	2886/2960 (98%)	2771 (96%)	113 (4%)	2 (0%)	53	70

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%)	32	49
1	B	654/662 (99%)	620 (95%)	34 (5%)	25	41
1	C	649/662 (98%)	616 (95%)	33 (5%)	26	42
1	D	648/662 (98%)	625 (96%)	23 (4%)	39	59
All	All	2602/2648 (98%)	2484 (96%)	118 (4%)	30	47

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	2.19	3 (12%)	31,47,47	1.90	9 (29%)
3	NAG	A	801	1	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
3	NAG	A	802	1	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
3	NAG	A	803	1	14,14,15	0.52	0	17,19,21	0.88	0
3	NAG	A	804	1,3	14,14,15	0.65	0	17,19,21	1.20	1 (5%)
3	NAG	A	805	3	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
3	NAG	A	806	1,3	14,14,15	0.49	0	17,19,21	1.31	2 (11%)
3	NAG	A	807	3	14,14,15	0.51	0	17,19,21	0.76	0
3	NAG	A	808	1	14,14,15	0.54	0	17,19,21	1.13	2 (11%)
2	XIH	B	800	-	24,32,32	2.18	3 (12%)	31,47,47	1.84	9 (29%)
3	NAG	B	801	1	14,14,15	0.69	0	17,19,21	1.66	3 (17%)
3	NAG	B	802	1	14,14,15	0.52	0	17,19,21	1.49	1 (5%)
3	NAG	B	803	1	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
3	NAG	B	804	1,3	14,14,15	0.58	0	17,19,21	0.93	0
3	NAG	B	805	3	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
3	NAG	B	806	1	14,14,15	0.49	0	17,19,21	1.49	4 (23%)
2	XIH	C	800	-	24,32,32	2.41	4 (16%)	31,47,47	1.88	11 (35%)
3	NAG	C	801	1	14,14,15	0.61	0	17,19,21	1.04	1 (5%)
3	NAG	C	802	1	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
3	NAG	C	803	1,3	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
3	NAG	C	804	3	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
3	NAG	C	805	1	14,14,15	0.61	0	17,19,21	1.10	1 (5%)
3	NAG	C	806	1	14,14,15	0.52	0	17,19,21	0.97	0
2	XIH	D	800	-	24,32,32	2.41	3 (12%)	31,47,47	1.60	6 (19%)
3	NAG	D	801	1	14,14,15	0.56	0	17,19,21	1.03	2 (11%)
3	NAG	D	802	1,3	14,14,15	0.47	0	17,19,21	1.08	2 (11%)
3	NAG	D	803	3	14,14,15	0.46	0	17,19,21	1.04	1 (5%)
3	NAG	D	804	1	14,14,15	0.61	0	17,19,21	1.46	3 (17%)

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	-9.76	1.29	1.44
2	D	800	XIH	C23-C24	-9.73	1.29	1.44
2	B	800	XIH	C23-C24	-9.12	1.30	1.44
2	A	800	XIH	C23-C24	-8.83	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	4.00	1.47	1.41
2	C	800	XIH	C3-C5	4.66	1.48	1.41
2	A	800	XIH	C3-C5	4.95	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	XIH	C3-C5	5.20	1.49	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	XIH	C3-C5-C6	-3.98	117.30	119.93
3	A	804	NAG	O5-C1-C2	-3.45	106.75	111.52
2	C	800	XIH	C11-C12-C13	-3.19	107.73	111.97
2	D	800	XIH	C3-C5-C6	-2.98	117.96	119.93
3	A	806	NAG	O5-C1-C2	-2.96	107.43	111.52
2	C	800	XIH	C3-C5-C6	-2.84	118.05	119.93
2	D	800	XIH	C10-N9-C8	-2.69	115.95	121.81
2	C	800	XIH	C17-C18-C19	-2.61	114.99	121.04
3	D	802	NAG	O5-C1-C2	-2.51	108.06	111.52
2	A	800	XIH	C17-C18-C19	-2.46	115.36	121.04
2	B	800	XIH	C10-N9-C8	-2.44	116.48	121.81
2	B	800	XIH	C3-C5-C6	-2.38	118.36	119.93
2	C	800	XIH	C10-N9-C8	-2.29	116.81	121.81
3	B	806	NAG	C4-C3-C2	-2.28	107.68	111.02
2	B	800	XIH	C17-C18-C19	-2.13	116.12	121.04
3	C	804	NAG	O5-C1-C2	-2.09	108.64	111.52
2	A	800	XIH	C10-N9-C8	-2.03	117.38	121.81
3	A	808	NAG	O5-C1-C2	-2.03	108.72	111.52
3	B	806	NAG	C3-C4-C5	-2.02	106.63	110.24
2	D	800	XIH	C27-N26-C6	2.00	121.27	118.33
3	D	801	NAG	C1-O5-C5	2.02	114.96	112.19
3	D	802	NAG	C1-O5-C5	2.05	115.01	112.19
3	D	801	NAG	C4-C3-C2	2.08	114.07	111.02
2	D	800	XIH	C17-C18-C23	2.16	123.55	120.64
2	A	800	XIH	C19-C18-C23	2.17	120.02	117.60
2	B	800	XIH	C11-C10-N9	2.20	115.35	111.08
3	B	803	NAG	C1-O5-C5	2.20	115.21	112.19
2	B	800	XIH	C27-N26-C6	2.26	121.65	118.33
2	C	800	XIH	C12-C11-C10	2.26	113.84	110.95
2	C	800	XIH	C18-C23-C24	2.29	122.56	120.24
3	A	801	NAG	C1-O5-C5	2.32	115.39	112.19
3	C	802	NAG	C4-C3-C2	2.34	114.44	111.02
3	C	803	NAG	C4-C3-C2	2.35	114.46	111.02
3	B	805	NAG	O5-C1-C2	2.36	114.78	111.52
3	B	806	NAG	O5-C5-C6	2.41	110.96	107.15
2	C	800	XIH	C19-C18-C23	2.47	120.36	117.60
3	B	801	NAG	O5-C1-C2	2.47	114.94	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	XIH	C13-C15-N9	2.55	112.94	109.96
3	D	804	NAG	O5-C1-C2	2.56	115.05	111.52
3	D	803	NAG	C1-O5-C5	2.61	115.78	112.19
3	C	801	NAG	C1-O5-C5	2.64	115.82	112.19
3	A	806	NAG	C1-O5-C5	2.69	115.89	112.19
2	A	800	XIH	C13-C15-N9	2.83	113.27	109.96
3	D	804	NAG	C1-O5-C5	2.87	116.13	112.19
3	C	805	NAG	C1-O5-C5	2.88	116.15	112.19
2	C	800	XIH	C17-C18-C23	2.93	124.59	120.64
2	A	800	XIH	C17-C18-C23	2.94	124.61	120.64
3	A	802	NAG	C1-O5-C5	2.99	116.31	112.19
2	B	800	XIH	C17-C18-C23	3.03	124.72	120.64
3	D	804	NAG	C4-C3-C2	3.09	115.55	111.02
2	A	800	XIH	C18-C23-C24	3.13	123.41	120.24
2	B	800	XIH	C18-C23-C24	3.24	123.52	120.24
3	A	805	NAG	C1-O5-C5	3.30	116.73	112.19
3	A	808	NAG	C1-O5-C5	3.36	116.81	112.19
3	B	801	NAG	C4-C3-C2	3.38	115.97	111.02
2	C	800	XIH	C10-N9-C15	3.55	123.47	112.74
2	D	800	XIH	C10-N9-C15	3.84	124.33	112.74
2	A	800	XIH	C10-N9-C15	3.88	124.45	112.74
3	B	801	NAG	O5-C5-C6	3.88	113.30	107.15
2	A	800	XIH	C18-C17-N16	3.90	119.78	113.31
2	B	800	XIH	C10-N9-C15	3.94	124.64	112.74
2	B	800	XIH	C18-C17-N16	3.95	119.87	113.31
3	B	806	NAG	C1-O5-C5	3.96	117.64	112.19
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	112.19
3	B	802	NAG	C1-O5-C5	4.86	118.88	112.19

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	723/740 (97%)	0.64	62 (8%) 10 9	39, 48, 74, 104	0
1	B	728/740 (98%)	0.49	47 (6%) 19 17	36, 49, 72, 93	0
1	C	723/740 (97%)	0.73	83 (11%) 5 4	39, 49, 73, 93	0
1	D	723/740 (97%)	1.07	138 (19%) 1 0	38, 54, 82, 118	0
All	All	2897/2960 (97%)	0.73	330 (11%) 5 4	36, 50, 76, 118	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	7.6
1	A	81	ALA	7.5
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	6.4
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	C	93	SER	5.4
1	A	95	PHE	5.4
1	D	372	TYR	5.4
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	D	135	TYR	5.1
1	C	76	ILE	5.1
1	C	88	VAL	5.1
1	D	81	ALA	5.0
1	B	78	VAL	4.9
1	D	386	TYR	4.9
1	D	98	PHE	4.9
1	D	464	GLU	4.9
1	D	148	ILE	4.9
1	D	93	SER	4.8
1	D	138	ASN	4.8
1	D	141	GLN	4.8
1	C	97	GLU	4.8
1	D	391	LYS	4.7
1	A	90	LEU	4.7
1	D	62	TRP	4.6
1	C	87	SER	4.6
1	D	468	TYR	4.6
1	C	90	LEU	4.6
1	D	335	GLY	4.6
1	D	78	VAL	4.5
1	D	442	VAL	4.5
1	D	392	LYS	4.4
1	A	140	ARG	4.4
1	C	330	TYR	4.4
1	A	93	SER	4.4
1	C	96	ASP	4.4
1	C	95	PHE	4.3
1	D	140	ARG	4.3
1	A	141	GLN	4.3
1	D	330	TYR	4.3
1	D	414	TYR	4.3
1	C	98	PHE	4.2
1	A	332	GLU	4.2
1	D	389	ILE	4.1
1	C	138	ASN	4.1
1	B	70	TYR	4.1
1	D	105	TYR	4.1
1	D	332	GLU	4.0
1	A	88	VAL	4.0
1	C	86	SER	4.0
1	D	395	THR	4.0

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

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

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Mol	Chain	Res	Type	RSRZ
1	D	444	CYS	2.9
1	C	81	ALA	2.9
1	A	547	TYR	2.9
1	D	413	ASP	2.8
1	B	628	GLY	2.8
1	B	630	SER	2.8
1	C	94	THR	2.8
1	C	114	ILE	2.8
1	D	342	ALA	2.8
1	D	328	CYS	2.8
1	B	547	TYR	2.8
1	C	105	TYR	2.8
1	D	334	SER	2.8
1	D	441	LYS	2.8
1	D	95	PHE	2.8
1	B	546	VAL	2.8
1	B	733	MET	2.8
1	C	75	ASN	2.8
1	D	489	LYS	2.8
1	C	283	THR	2.8
1	C	335	GLY	2.7
1	C	490	GLY	2.7
1	B	90	LEU	2.7
1	C	142	LEU	2.7
1	C	332	GLU	2.7
1	D	400	GLY	2.7
1	C	79	PHE	2.7
1	D	412	SER	2.7
1	D	435	GLN	2.7
1	B	140	ARG	2.7
1	D	173	TYR	2.7
1	D	344	GLN	2.7
1	D	629	TRP	2.7
1	D	431	LEU	2.7
1	D	287	ILE	2.7
1	D	742	ILE	2.7
1	C	102	ILE	2.7
1	B	631	TYR	2.7
1	D	394	CYS	2.7
1	D	179	ASN	2.7
1	D	72	GLN	2.7
1	B	142	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	666	TYR	2.6
1	C	70	TYR	2.6
1	D	114	ILE	2.6
1	D	703	ILE	2.6
1	D	336	ARG	2.6
1	C	388	GLN	2.6
1	D	434	ILE	2.6
1	A	105	TYR	2.6
1	B	138	ASN	2.6
1	B	357	PHE	2.6
1	D	269	PHE	2.6
1	B	521	GLU	2.6
1	D	61	ARG	2.6
1	C	210	ALA	2.6
1	D	486	VAL	2.6
1	C	99	GLY	2.6
1	C	54	ARG	2.6
1	A	145	GLU	2.6
1	C	91	GLU	2.6
1	D	384	ILE	2.6
1	B	87	SER	2.5
1	B	711	VAL	2.5
1	D	343	ARG	2.5
1	D	390	ASP	2.5
1	B	71	LYS	2.5
1	C	653	VAL	2.5
1	C	333	SER	2.5
1	C	140	ARG	2.5
1	D	378	GLU	2.5
1	D	521	GLU	2.5
1	B	703	ILE	2.5
1	C	145	GLU	2.5
1	D	388	GLN	2.5
1	D	487	ASN	2.5
1	D	462	SER	2.5
1	D	285	ILE	2.5
1	D	223	LEU	2.5
1	C	392	LYS	2.4
1	D	85	ASN	2.4
1	C	711	VAL	2.4
1	A	330	TYR	2.4
1	D	63	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	488	ASP	2.4
1	D	409	ALA	2.4
1	C	181	PRO	2.4
1	D	443	THR	2.4
1	D	653	VAL	2.4
1	A	552	SER	2.4
1	A	740	HIS	2.4
1	C	209	SER	2.4
1	C	278	SER	2.4
1	B	705	GLY	2.4
1	B	139	LYS	2.3
1	D	630	SER	2.4
1	C	147	ARG	2.3
1	D	766	PRO	2.3
1	D	469	GLN	2.3
1	B	518	ILE	2.3
1	C	132	TYR	2.3
1	D	86	SER	2.3
1	C	208	PHE	2.3
1	A	666	TYR	2.3
1	C	118	TYR	2.3
1	B	99	GLY	2.3
1	A	143	ILE	2.3
1	B	205	GLU	2.3
1	A	142	LEU	2.3
1	D	187	TRP	2.3
1	D	734	TRP	2.3
1	B	86	SER	2.3
1	C	537	SER	2.3
1	A	357	PHE	2.3
1	D	402	TRP	2.3
1	A	399	LYS	2.3
1	D	136	ASP	2.3
1	A	148	ILE	2.3
1	A	336	ARG	2.2
1	A	166	TYR	2.2
1	D	160	VAL	2.2
1	B	210	ALA	2.2
1	B	505	GLN	2.2
1	A	144	THR	2.2
1	B	755	MET	2.2
1	D	422	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	LYS	2.2
1	C	41	LYS	2.2
1	D	656	VAL	2.2
1	C	650	GLY	2.2
1	A	201	TRP	2.2
1	B	63	ILE	2.2
1	C	505	GLN	2.2
1	D	399	LYS	2.2
1	A	274	ASP	2.2
1	B	84	GLY	2.2
1	A	208	PHE	2.2
1	A	210	ALA	2.2
1	C	139	LYS	2.2
1	C	651	ILE	2.2
1	C	504	LEU	2.1
1	D	477	LEU	2.1
1	B	141	GLN	2.1
1	A	54	ARG	2.1
1	D	329	ASP	2.1
1	A	85	ASN	2.1
1	A	506	ASN	2.1
1	A	630	SER	2.1
1	D	164	LEU	2.1
1	D	340	LEU	2.1
1	D	530	LEU	2.1
1	C	536	LYS	2.1
1	B	442	VAL	2.1
1	B	467	TYR	2.1
1	C	713	PHE	2.1
1	C	276	LEU	2.1
1	C	702	LEU	2.1
1	A	162	HIS	2.1
1	B	328	CYS	2.1
1	D	147	ARG	2.1
1	C	487	ASN	2.1
1	D	219	ASN	2.1
1	C	666	TYR	2.1
1	A	502	LYS	2.1
1	A	632	GLY	2.1
1	B	627	TRP	2.1
1	B	76	ILE	2.0
1	A	707	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	652	ALA	2.0
1	A	546	VAL	2.0
1	B	708	ASP	2.0
1	D	305	TRP	2.0
1	A	77	LEU	2.0
1	A	102	ILE	2.0
1	B	702	LEU	2.0
1	C	280	THR	2.0
1	A	181	PRO	2.0
1	A	665	VAL	2.0
1	B	558	VAL	2.0
1	A	670	TYR	2.0
1	C	187	TRP	2.0
1	C	63	ILE	2.0
1	C	143	ILE	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	801	14/15	0.62	0.29	95,95,96,96	0
3	NAG	A	802	14/15	0.66	0.30	75,78,79,79	0
3	NAG	B	801	14/15	0.68	0.16	79,80,81,81	0
3	NAG	C	805	14/15	0.69	0.20	78,81,82,82	0
3	NAG	A	806	14/15	0.70	0.20	80,84,85,87	0
3	NAG	B	806	14/15	0.72	0.14	69,71,74,74	0
3	NAG	C	801	14/15	0.74	0.20	60,60,61,62	0
3	NAG	D	804	14/15	0.77	0.13	81,83,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	803	14/15	0.79	0.21	69,72,76,77	0
3	NAG	B	803	14/15	0.80	0.24	64,67,70,71	0
3	NAG	A	807	14/15	0.81	0.20	90,91,92,92	0
3	NAG	A	805	14/15	0.83	0.14	67,68,69,69	0
3	NAG	C	806	14/15	0.84	0.21	68,73,74,74	0
3	NAG	B	805	14/15	0.84	0.26	77,79,80,80	0
3	NAG	D	801	14/15	0.85	0.18	65,67,68,69	0
3	NAG	B	802	14/15	0.85	0.16	67,68,69,70	0
3	NAG	C	804	14/15	0.87	0.18	73,75,77,77	0
3	NAG	C	802	14/15	0.87	0.15	70,72,75,75	0
3	NAG	D	803	14/15	0.87	0.12	73,75,76,77	0
3	NAG	B	804	14/15	0.91	0.19	62,65,69,73	0
3	NAG	C	803	14/15	0.92	0.14	60,63,66,70	0
3	NAG	A	804	14/15	0.93	0.17	56,59,62,65	0
3	NAG	D	802	14/15	0.93	0.12	60,63,65,69	0
3	NAG	A	808	14/15	0.94	0.18	62,66,68,68	0
2	XIH	B	800	29/29	0.96	0.27	35,39,40,41	0
2	XIH	D	800	29/29	0.96	0.23	40,42,43,45	0
2	XIH	A	800	29/29	0.97	0.28	38,43,44,44	0
2	XIH	C	800	29/29	0.97	0.23	35,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.