



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 06:43 PM EDT

PDB ID : 3CCB
Title : Crystal Structure of Human DPP4 in complex with a benzimidazole derivative
Authors : Wallace, M.B.; Skene, R.J.
Deposited on : unknown
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

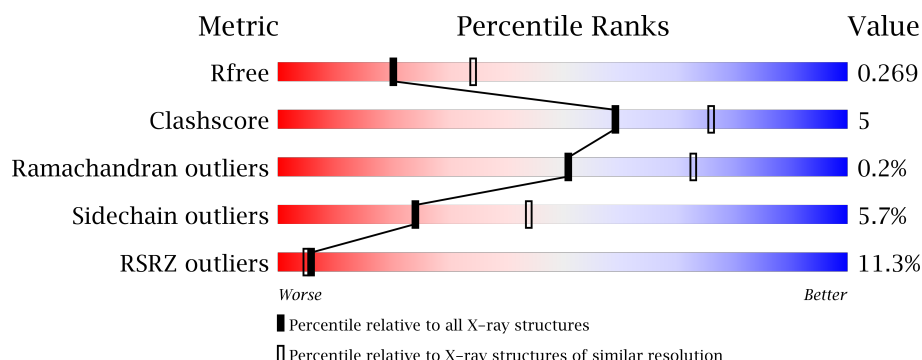
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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>11%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	740	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	740	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	740	<div> <div>16%</div> <div> <div></div> <div>81%</div> <div>15%</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
2	NAG	A	808	-	-	-	X
2	NAG	C	802	-	-	-	X
2	NAG	D	804	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24805 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	724	Total	C	N	O	S	0	1	0
			5935	3812	977	1120	26			
1	B	729	Total	C	N	O	S	0	0	0
			5965	3830	983	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5936	3813	977	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



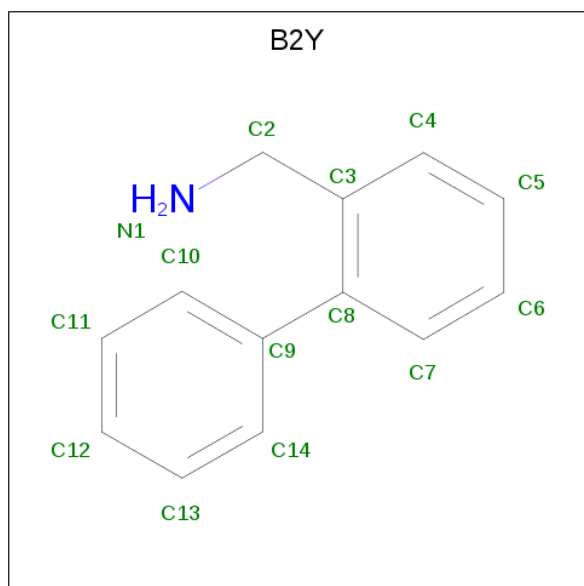
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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

- Molecule 3 is 1-biphenyl-2-ylmethanamine (three-letter code: B2Y) (formula: C₁₃H₁₃N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	13	1		
3	B	1	Total	C	N	0	0
			14	13	1		
3	C	1	Total	C	N	0	0
			14	13	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	N	0	0
			14	13	1		

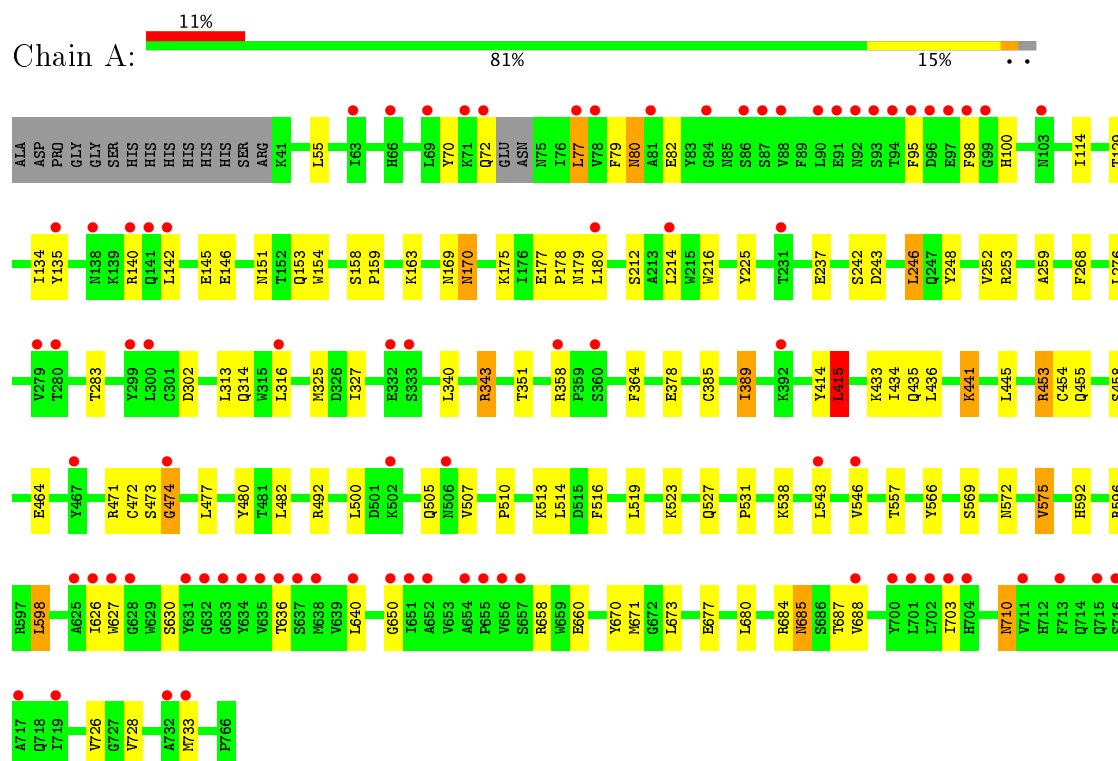
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	191	Total	O	0	0
			191	191		
4	C	189	Total	O	0	0
			189	189		
4	D	90	Total	O	0	0
			90	90		

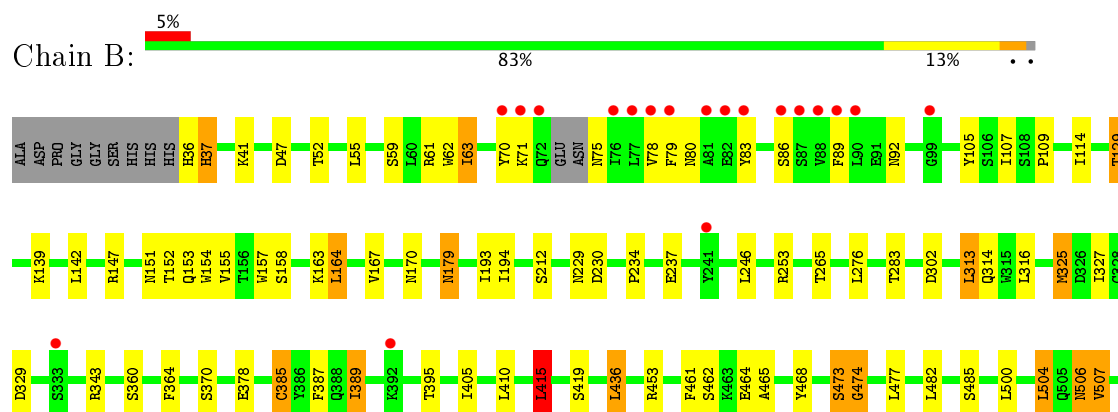
3 Residue-property plots [i](#)

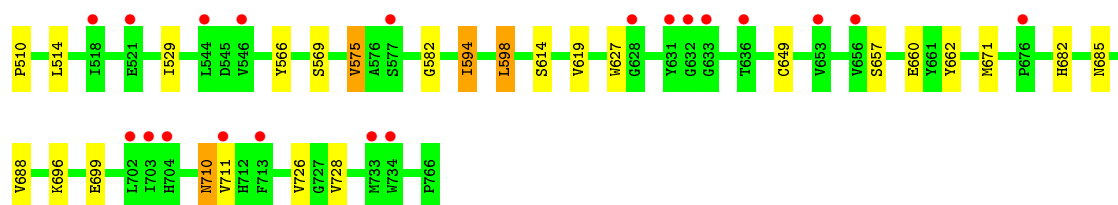
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

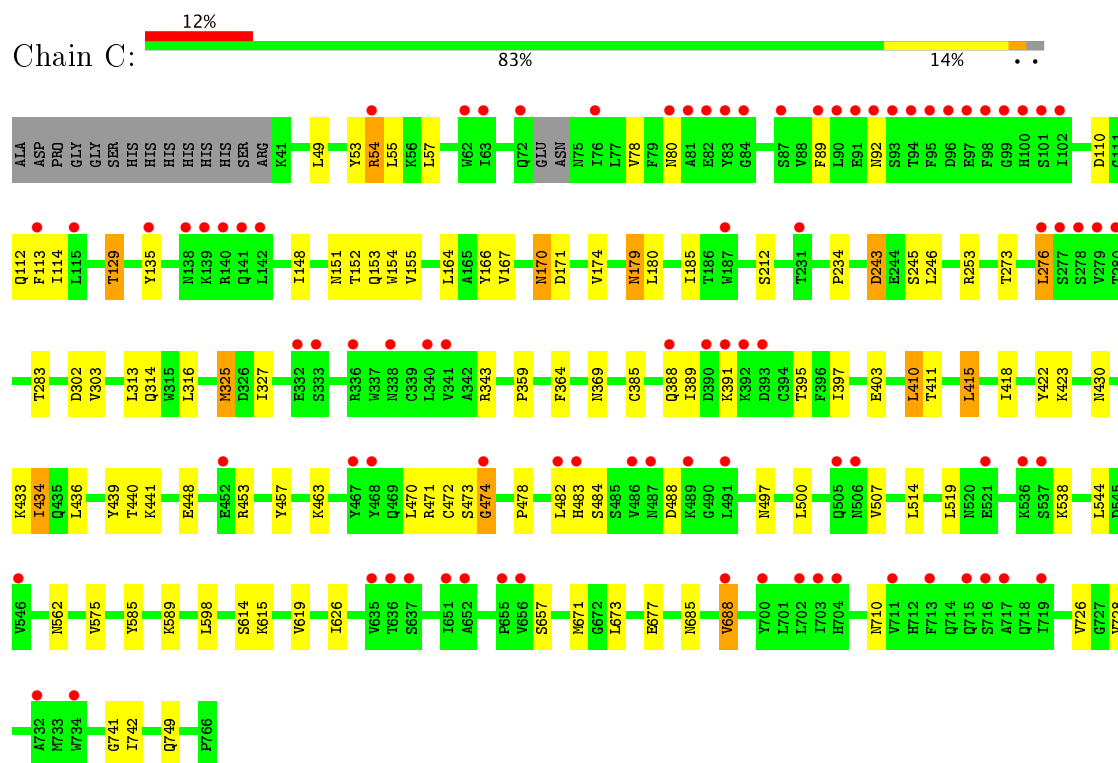


- Molecule 1: Dipeptidyl peptidase 4

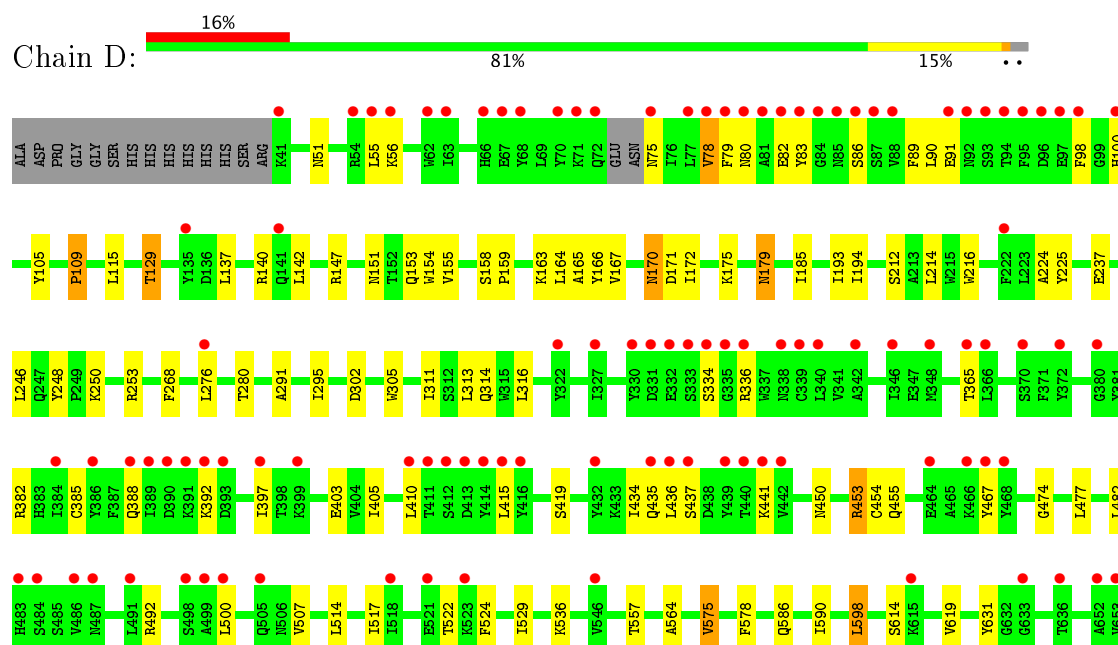


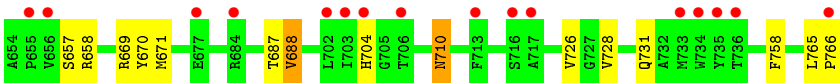


• Molecule 1: Dipeptidyl peptidase 4



• 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	122.09Å 123.01Å 144.65Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	32.80 – 2.49 32.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.80-2.49) 98.3 (32.82-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.244 0.233 , 0.269	Depositor DCC
R_{free} test set	6729 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24805	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, B2Y

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	0/6111	0.62	1/8311 (0.0%)
1	B	0.44	0/6138	0.62	1/8348 (0.0%)
1	C	0.44	0/6111	0.61	1/8311 (0.0%)
1	D	0.42	0/6100	0.58	0/8296
All	All	0.44	0/24460	0.61	3/33266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	415	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	415	LEU	CA-CB-CG	5.13	127.11	115.30

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	5935	0	5657	72	0
1	B	5965	0	5672	63	0
1	C	5936	0	5660	65	0
1	D	5929	0	5651	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	112	0	102	0	0
2	B	84	0	77	2	0
2	C	56	0	51	0	0
2	D	56	0	51	1	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	206	0	0	2	0
4	B	191	0	0	0	0
4	C	189	0	0	1	0
4	D	90	0	0	0	0
All	All	24805	0	22973	253	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 5.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.42	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.14	0.93
1:A:153:GLN:HE22	1:A:170:ASN:H	1.18	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.14	0.90
1:C:54:ARG:HH21	1:C:54:ARG:HG2	1.39	0.88
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.56	0.88
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.71	0.87
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.58	0.85
1:D:153:GLN:HE22	1:D:170:ASN:H	1.22	0.84
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.88	0.83
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.59	0.82
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.82
1:A:325:MET:CE	1:A:327:ILE:HD11	2.11	0.81
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.64	0.79
1:C:434:ILE:HD11	1:C:439:TYR:HB2	1.67	0.74
1:A:129:THR:HG23	1:A:151:ASN:HA	1.70	0.73
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.73	0.70
1:D:179:ASN:HD22	1:D:179:ASN:H	1.42	0.67
1:A:129:THR:CG2	1:A:151:ASN:HA	2.25	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.92	0.64
1:B:36:HIS:O	1:B:37:HIS:HB2	1.98	0.63
1:B:614:SER:HA	1:B:619:VAL:HB	1.79	0.63
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.63
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.80	0.62
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.23	0.62
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.82	0.62
1:C:153:GLN:NE2	1:C:170:ASN:H	1.94	0.62
1:D:147:ARG:HE	2:D:801:NAG:H83	1.66	0.61
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.65	0.61
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.61
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.36	0.60
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.92	0.60
1:D:564:ALA:HB1	1:D:575:VAL:HG11	1.84	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:D:155:VAL:HG12	1:D:166:TYR:HB3	1.85	0.59
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.85	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:B:711:VAL:CG2	3:B:800:B2Y:H11	2.32	0.58
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.84	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.58
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.84	0.58
1:C:472:CYS:O	1:C:478:PRO:HA	2.04	0.57
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.67	0.57
1:D:522:THR:HB	1:D:524:PHE:CE2	2.40	0.57
1:D:382:ARG:H	1:D:403:GLU:HG2	1.69	0.57
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.86	0.57
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.86	0.56
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.87	0.56
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.40	0.56
1:C:152:THR:HG21	1:C:155:VAL:HG13	1.88	0.55
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.88	0.55
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.71	0.55
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.89	0.55
1:D:78:VAL:HG22	1:D:89:PHE:HB2	1.88	0.55
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.42	0.54
1:C:153:GLN:HE22	1:C:170:ASN:N	1.95	0.54
1:B:343:ARG:HD3	1:B:389:ILE:CG2	2.32	0.54
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.54
1:B:89:PHE:HE1	1:B:107:ILE:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.54
1:D:614:SER:HA	1:D:619:VAL:HB	1.89	0.53
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.74	0.53
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.89	0.53
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.39	0.53
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.90	0.52
1:A:135:TYR:HE2	1:A:140:ARG:HG2	1.74	0.52
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.52
1:A:170:ASN:N	1:A:170:ASN:HD22	2.08	0.51
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.92	0.51
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.40	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.91	0.51
1:B:179:ASN:H	1:B:179:ASN:HD22	1.57	0.51
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.51
1:B:147:ARG:HE	2:B:802:NAG:H83	1.75	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.46	0.51
1:D:453:ARG:NH2	1:D:477:LEU:O	2.43	0.51
1:C:369:ASN:C	1:C:389:ILE:HG12	2.32	0.51
1:C:369:ASN:O	1:C:389:ILE:HG12	2.11	0.50
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.50
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.27	0.50
1:D:598:LEU:HG	1:D:631:TYR:OH	2.12	0.49
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.93	0.49
1:D:334:SER:HB2	1:D:336:ARG:H	1.77	0.49
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.49
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.49
1:C:54:ARG:NH2	1:C:54:ARG:HG2	2.16	0.49
1:B:79:PHE:HA	1:B:86:SER:HB3	1.94	0.49
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.49
1:B:47:ASP:HA	1:B:52:THR:OG1	2.12	0.49
1:B:80:ASN:HD22	1:B:83:TYR:H	1.59	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.13	0.49
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.13	0.49
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.13	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.93	0.48
1:C:327:ILE:HD13	1:C:389:ILE:HG23	1.95	0.48
1:D:75:ASN:OD1	1:D:91:GLU:HG3	2.12	0.48
1:C:473:SER:O	1:C:474:GLY:O	2.32	0.48
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.95	0.48
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.48
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.14	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.47
1:B:473:SER:O	1:B:474:GLY:O	2.32	0.47
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.13	0.47
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.48	0.47
1:B:71:LYS:HA	1:B:75:ASN:O	2.14	0.47
1:C:179:ASN:HD22	1:C:179:ASN:C	2.18	0.47
1:A:153:GLN:HE22	1:A:170:ASN:N	2.00	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.96	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
2:B:804:NAG:H62	2:B:805:NAG:N2	2.30	0.47
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.49	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.96	0.47
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.80	0.47
1:D:80:ASN:HD22	1:D:83:TYR:HB2	1.80	0.47
1:D:435:GLN:HE21	1:D:437:SER:HG	1.63	0.47
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.47
1:C:303:VAL:HG22	1:C:313:LEU:HD12	1.97	0.47
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.49	0.46
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.97	0.46
1:D:158:SER:OG	1:D:163:LYS:HB2	2.15	0.46
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.46
1:A:685:ASN:ND2	4:A:866:HOH:O	2.48	0.46
1:D:710:ASN:C	1:D:710:ASN:HD22	2.19	0.46
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.97	0.46
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.98	0.46
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.46
1:C:55:LEU:HD23	1:C:500:LEU:HD22	1.98	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.98	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.98	0.46
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.31	0.45
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.80	0.45
1:D:405:ILE:HG12	1:D:419:SER:HA	1.98	0.45
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.45
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.98	0.45
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.45
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.52	0.45
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.45
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.47	0.45
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.82	0.45
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.45
1:C:410:LEU:HD22	1:C:411:THR:O	2.16	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.52	0.45
1:B:153:GLN:NE2	1:B:170:ASN:H	2.06	0.45
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.94	0.45
1:D:129:THR:HG23	1:D:151:ASN:HA	1.98	0.45
1:D:731:GLN:HG3	1:D:758:PHE:HE1	1.82	0.44
1:A:135:TYR:CE2	1:A:140:ARG:HA	2.52	0.44
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.99	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.44
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.15	0.44
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.44
1:C:614:SER:HA	1:C:619:VAL:HB	2.00	0.44
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.52	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.00	0.44
1:B:378:GLU:H	1:B:378:GLU:CD	2.21	0.44
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.82	0.44
1:B:75:ASN:HD21	1:B:92:ASN:HD22	1.66	0.43
1:D:517:ILE:HD11	1:D:578:PHE:CE1	2.53	0.43
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.54	0.43
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.00	0.43
1:B:405:ILE:HG12	1:B:419:SER:HA	2.00	0.43
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.01	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:C:544:LEU:HD23	1:C:626:ILE:HD12	2.00	0.43
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.54	0.43
1:A:473:SER:O	1:A:474:GLY:O	2.36	0.43
1:D:291:ALA:O	1:D:295:ILE:HG23	2.18	0.43
1:A:596:ARG:HA	1:A:670:TYR:O	2.19	0.43
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.54	0.43
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.54	0.43
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.54	0.43
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.58	0.43
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.53	0.43
1:C:148:ILE:HD11	1:C:164:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.49	0.42
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.54	0.42
1:A:72:GLN:HB2	1:A:77:LEU:HD21	2.01	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.42
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.54	0.42
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.42
1:C:418:ILE:HA	1:C:430:ASN:O	2.19	0.42
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.19	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:A:129:THR:HG22	4:A:1002:HOH:O	2.18	0.42
1:C:155:VAL:HG12	1:C:166:TYR:HB3	2.01	0.42
1:D:450:ASN:O	1:D:454:CYS:HB2	2.20	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.42
1:C:179:ASN:HD22	1:C:180:LEU:N	2.17	0.42
1:D:435:GLN:OE1	1:D:441:LYS:HD3	2.19	0.42
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.91	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.41
1:B:70:TYR:CG	1:B:71:LYS:N	2.88	0.41
1:C:167:VAL:HA	1:C:171:ASP:O	2.20	0.41
1:C:302:ASP:HB3	1:C:314:GLN:HB2	2.01	0.41
1:A:378:GLU:CD	1:A:378:GLU:H	2.23	0.41
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.41
1:C:397:ILE:HD12	1:C:434:ILE:HD13	2.03	0.41
1:B:506:ASN:HB2	1:C:440:THR:CG2	2.49	0.41
1:D:98:PHE:CD1	1:D:100:HIS:HB2	2.55	0.41
1:D:79:PHE:CD2	1:D:86:SER:HB3	2.54	0.41
1:A:458:SER:OG	1:A:471:ARG:HB3	2.21	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.55	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:D:598:LEU:HB2	1:D:671:MET:SD	2.60	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.56	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.20	0.41
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.56	0.41
1:A:135:TYR:CE2	1:A:140:ARG:HG2	2.55	0.41
1:C:478:PRO:HB2	1:C:497:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HD23	1:D:500:LEU:HD22	2.02	0.41
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.02	0.41
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.41
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.03	0.41
1:A:242:SER:OG	1:A:243:ASP:N	2.53	0.41
1:D:167:VAL:HA	1:D:171:ASP:O	2.21	0.41
1:A:146:GLU:O	1:A:175:LYS:NZ	2.52	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HG	2.02	0.41
1:A:154:TRP:CD2	1:A:212:SER:HB3	2.56	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.51	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.77	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:B:598:LEU:O	1:B:682:HIS:NE2	2.52	0.41
1:C:562:ASN:HB2	4:C:841:HOH:O	2.20	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.22	0.41
1:B:582:GLY:CA	1:B:594:ILE:HD12	2.50	0.40
1:C:484:SER:O	1:C:488:ASP:HA	2.20	0.40
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.51	0.40
1:A:158:SER:OG	1:A:163:LYS:HB2	2.22	0.40
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:A:546:VAL:HG12	1:A:627:TRP:O	2.21	0.40
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.40
1:D:164:LEU:HB3	1:D:175:LYS:HB2	2.03	0.40
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.57	0.40
1:B:63:ILE:HA	1:B:63:ILE:HD12	1.81	0.40
1:C:243:ASP:C	1:C:245:SER:N	2.75	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	721/740 (97%)	684 (95%)	36 (5%)	1 (0%)	55	76
1	B	725/740 (98%)	698 (96%)	25 (3%)	2 (0%)	44	66
1	C	721/740 (97%)	688 (95%)	31 (4%)	2 (0%)	44	66
1	D	720/740 (97%)	684 (95%)	34 (5%)	2 (0%)	44	66
All	All	2887/2960 (98%)	2754 (95%)	126 (4%)	7 (0%)	51	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	GLY
1	A	474	GLY
1	B	37	HIS
1	B	474	GLY
1	D	474	GLY
1	C	92	ASN
1	D	109	PRO

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	650/662 (98%)	611 (94%)	39 (6%)	22	41
1	B	652/662 (98%)	611 (94%)	41 (6%)	21	38
1	C	650/662 (98%)	614 (94%)	36 (6%)	25	46
1	D	649/662 (98%)	617 (95%)	32 (5%)	29	52
All	All	2601/2648 (98%)	2453 (94%)	148 (6%)	24	44

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	80	ASN
1	A	95	PHE
1	A	145	GLU

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	343	ARG
1	A	358[A]	ARG
1	A	358[B]	ARG
1	A	385	CYS
1	A	389	ILE
1	A	415	LEU
1	A	436	LEU
1	A	441	LYS
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	566	TYR
1	A	575	VAL
1	A	598	LEU
1	A	630	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	129	THR
1	B	139	LYS
1	B	142	LEU

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Mol	Chain	Res	Type
1	B	164	LEU
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	316	LEU
1	B	325	MET
1	B	360	SER
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	464	GLU
1	B	473	SER
1	B	477	LEU
1	B	482	LEU
1	B	504	LEU
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	566	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	627	TRP
1	B	660	GLU
1	B	685	ASN
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	80	ASN
1	C	129	THR
1	C	170	ASN
1	C	179	ASN
1	C	243	ASP
1	C	246	LEU

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Mol	Chain	Res	Type
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET
1	C	385	CYS
1	C	395	THR
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	434	ILE
1	C	436	LEU
1	C	441	LYS
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	538	LYS
1	C	575	VAL
1	C	589	LYS
1	C	615	LYS
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	D	51	ASN
1	D	56	LYS
1	D	78	VAL
1	D	90	LEU
1	D	109	PRO
1	D	129	THR
1	D	137	LEU
1	D	140	ARG
1	D	142	LEU
1	D	170	ASN
1	D	179	ASN
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU

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Mol	Chain	Res	Type
1	D	280	THR
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	482	LEU
1	D	492	ARG
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	575	VAL
1	D	598	LEU
1	D	688	VAL
1	D	704	HIS
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	80	ASN
1	B	92	ASN
1	B	123	GLN
1	B	138	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	430	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	51	ASN
1	C	80	ASN
1	C	100	HIS
1	C	123	GLN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	505	GLN
1	C	697	GLN
1	C	710	ASN
1	C	748	HIS
1	D	80	ASN
1	D	138	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	430	ASN
1	D	455	GLN
1	D	508	GLN
1	D	572	ASN
1	D	592	HIS
1	D	621	ASN
1	D	710	ASN
1	D	748	HIS

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 ⓘ

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	B2Y	A	800	-	15,15,15	0.47	0	19,19,19	0.76	0
2	NAG	A	801	1	14,14,15	0.57	0	15,19,21	1.49	1 (6%)
2	NAG	A	802	1	14,14,15	0.56	0	15,19,21	1.44	1 (6%)
2	NAG	A	803	1	14,14,15	0.58	0	15,19,21	1.03	1 (6%)
2	NAG	A	804	1,2	14,14,15	0.59	0	15,19,21	0.99	1 (6%)
2	NAG	A	805	2	14,14,15	0.45	0	15,19,21	1.01	0
2	NAG	A	806	1,2	14,14,15	0.53	0	15,19,21	1.50	3 (20%)
2	NAG	A	807	2	14,14,15	0.56	0	15,19,21	0.84	0
2	NAG	A	808	1	14,14,15	0.56	0	15,19,21	1.44	1 (6%)
3	B2Y	B	800	-	15,15,15	0.48	0	19,19,19	0.59	0
2	NAG	B	801	1	14,14,15	0.76	1 (7%)	15,19,21	1.27	1 (6%)
2	NAG	B	802	1	14,14,15	0.51	0	15,19,21	1.20	1 (6%)
2	NAG	B	803	1	14,14,15	0.61	0	15,19,21	1.26	1 (6%)
2	NAG	B	804	1,2	14,14,15	0.63	0	15,19,21	0.98	0
2	NAG	B	805	2	14,14,15	0.52	0	15,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	806	1	14,14,15	0.54	0	15,19,21	1.65	1 (6%)
3	B2Y	C	800	-	15,15,15	0.46	0	19,19,19	0.74	0
2	NAG	C	801	1	14,14,15	0.48	0	15,19,21	1.44	1 (6%)
2	NAG	C	802	1	14,14,15	0.63	0	15,19,21	1.39	1 (6%)
2	NAG	C	803	1,2	14,14,15	0.62	0	15,19,21	0.94	0
2	NAG	C	804	2	14,14,15	0.62	0	15,19,21	1.35	2 (13%)
3	B2Y	D	800	-	15,15,15	0.45	0	19,19,19	0.64	0
2	NAG	D	801	1	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
2	NAG	D	802	1,2	14,14,15	0.44	0	15,19,21	1.09	1 (6%)
2	NAG	D	803	2	14,14,15	0.59	0	15,19,21	0.89	0
2	NAG	D	804	1	14,14,15	0.76	1 (7%)	15,19,21	1.62	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
3	B2Y	A	800	-	-	0/6/6/6	0/2/2/2
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	806	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	807	2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
3	B2Y	B	800	-	-	0/6/6/6	0/2/2/2
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
2	NAG	B	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	805	2	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	B2Y	C	800	-	-	0/6/6/6	0/2/2/2
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
2	NAG	C	803	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	804	2	-	0/6/23/26	0/1/1/1
3	B2Y	D	800	-	-	0/6/6/6	0/2/2/2
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	802	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	803	2	-	0/6/23/26	0/1/1/1
2	NAG	D	804	1	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAG	C1-C2	2.08	1.55	1.52
2	D	804	NAG	C1-C2	2.43	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	NAG	O5-C1-C2	-3.09	107.17	111.47
2	A	804	NAG	O5-C1-C2	-2.60	107.85	111.47
2	D	804	NAG	C3-C4-C5	-2.37	106.03	110.22
2	A	806	NAG	C2-N2-C7	-2.18	119.76	122.94
2	C	804	NAG	C3-C4-C5	2.22	114.13	110.22
2	D	802	NAG	C1-O5-C5	2.49	115.59	112.17
2	D	801	NAG	C1-O5-C5	2.60	115.75	112.17
2	A	803	NAG	C4-C3-C2	2.66	114.91	111.02
2	D	804	NAG	O5-C1-C2	2.83	115.41	111.47
2	A	806	NAG	C1-O5-C5	2.88	116.13	112.17
2	B	801	NAG	C4-C3-C2	3.27	115.81	111.02
2	D	804	NAG	C1-O5-C5	3.80	117.40	112.17
2	C	802	NAG	C4-C3-C2	3.80	116.59	111.02
2	C	804	NAG	C4-C3-C2	3.87	116.68	111.02
2	B	802	NAG	C1-O5-C5	3.94	117.60	112.17
2	B	803	NAG	C1-O5-C5	3.95	117.60	112.17
2	C	801	NAG	C1-O5-C5	4.37	118.19	112.17
2	A	808	NAG	C1-O5-C5	4.59	118.49	112.17
2	A	801	NAG	C1-O5-C5	4.77	118.75	112.17
2	A	802	NAG	C1-O5-C5	5.35	119.54	112.17
2	B	806	NAG	C1-O5-C5	5.61	119.89	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	804	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	B2Y	1	0
2	B	802	NAG	1	0
2	B	804	NAG	1	0
2	B	805	NAG	1	0
2	D	801	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	724/740 (97%)	0.60	81 (11%) 6 5	37, 48, 68, 104	0
1	B	729/740 (98%)	0.33	39 (5%) 27 28	36, 47, 67, 83	0
1	C	724/740 (97%)	0.65	87 (12%) 5 4	37, 48, 69, 101	0
1	D	724/740 (97%)	0.74	121 (16%) 2 1	36, 51, 69, 107	0
All	All	2901/2960 (98%)	0.58	328 (11%) 6 5	36, 48, 68, 107	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	8.3
1	D	83	TYR	7.9
1	C	135	TYR	7.6
1	C	279	VAL	7.1
1	D	93	SER	7.0
1	C	93	SER	6.4
1	D	94	THR	6.2
1	C	94	THR	6.0
1	C	99	GLY	5.6
1	A	92	ASN	5.6
1	A	88	VAL	5.4
1	D	77	LEU	5.4
1	A	135	TYR	5.3
1	D	386	TYR	5.2
1	C	96	ASP	5.0
1	D	414	TYR	4.9
1	A	140	ARG	4.8
1	C	83	TYR	4.7
1	C	92	ASN	4.6
1	C	141	GLN	4.6
1	C	280	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	SER	4.5
1	A	96	ASP	4.5
1	B	81	ALA	4.5
1	B	518	ILE	4.5
1	D	734	TRP	4.4
1	D	412	SER	4.4
1	B	88	VAL	4.4
1	D	88	VAL	4.4
1	D	330	TYR	4.3
1	D	333	SER	4.3
1	D	518	ILE	4.3
1	A	95	PHE	4.3
1	D	487	ASN	4.3
1	B	87	SER	4.2
1	B	86	SER	4.2
1	D	55	LEU	4.2
1	D	81	ALA	4.2
1	C	102	ILE	4.2
1	A	97	GLU	4.2
1	A	333	SER	4.2
1	D	97	GLU	4.2
1	A	635	VAL	4.1
1	C	187	TRP	4.1
1	C	81	ALA	4.1
1	A	332	GLU	4.0
1	A	702	LEU	4.0
1	D	78	VAL	4.0
1	D	441	LYS	4.0
1	B	70	TYR	4.0
1	D	505	GLN	3.9
1	A	138	ASN	3.9
1	C	392	LYS	3.8
1	C	340	LEU	3.8
1	A	98	PHE	3.7
1	D	334	SER	3.7
1	D	85	ASN	3.7
1	D	436	LEU	3.7
1	D	468	TYR	3.7
1	C	702	LEU	3.7
1	C	489	LYS	3.7
1	C	734	TRP	3.7
1	D	62	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	713	PHE	3.7
1	D	322	TYR	3.7
1	C	97	GLU	3.6
1	A	93	SER	3.6
1	D	498	SER	3.6
1	D	399	LYS	3.6
1	B	72	GLN	3.6
1	C	467	TYR	3.6
1	D	439	TYR	3.6
1	D	766	PRO	3.5
1	D	86	SER	3.5
1	D	435	GLN	3.5
1	A	700	TYR	3.5
1	D	467	TYR	3.5
1	D	413	ASP	3.5
1	D	486	VAL	3.5
1	A	69	LEU	3.5
1	D	366	LEU	3.5
1	A	636	THR	3.5
1	D	100	HIS	3.4
1	D	84	GLY	3.4
1	A	81	ALA	3.4
1	D	96	ASP	3.4
1	C	332	GLU	3.4
1	D	56	LYS	3.3
1	D	397	ILE	3.3
1	A	94	THR	3.3
1	A	651	ILE	3.3
1	C	487	ASN	3.3
1	A	634	TYR	3.3
1	C	474	GLY	3.2
1	B	546	VAL	3.2
1	A	713	PHE	3.2
1	A	655	PRO	3.2
1	C	390	ASP	3.2
1	A	652	ALA	3.2
1	A	656	VAL	3.2
1	A	279	VAL	3.1
1	D	340	LEU	3.1
1	D	706	THR	3.1
1	A	626	ILE	3.1
1	C	506	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	TYR	3.1
1	D	332	GLU	3.1
1	A	701	LEU	3.1
1	D	92	ASN	3.1
1	D	66	HIS	3.1
1	D	464	GLU	3.1
1	D	98	PHE	3.1
1	A	87	SER	3.1
1	C	732	ALA	3.1
1	C	719	ILE	3.0
1	C	652	ALA	3.0
1	A	719	ILE	3.0
1	A	637	SER	3.0
1	D	491	LEU	3.0
1	C	486	VAL	3.0
1	C	80	ASN	3.0
1	B	734	TRP	3.0
1	A	84	GLY	3.0
1	C	713	PHE	3.0
1	A	141	GLN	3.0
1	C	142	LEU	3.0
1	C	636	THR	3.0
1	B	90	LEU	2.9
1	B	83	TYR	2.9
1	D	331	ASP	2.9
1	A	703	ILE	2.9
1	A	716	SER	2.9
1	C	82	GLU	2.9
1	D	483	HIS	2.9
1	B	78	VAL	2.9
1	B	77	LEU	2.9
1	D	437	SER	2.9
1	C	717	ALA	2.9
1	C	536	LYS	2.9
1	B	89	PHE	2.8
1	D	652	ALA	2.8
1	A	627	TRP	2.8
1	D	466	LYS	2.8
1	D	80	ASN	2.8
1	C	98	PHE	2.8
1	D	91	GLU	2.8
1	D	615	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	327	ILE	2.8
1	A	732	ALA	2.8
1	C	505	GLN	2.8
1	D	702	LEU	2.8
1	C	656	VAL	2.7
1	D	521	GLU	2.7
1	D	372	TYR	2.7
1	C	716	SER	2.7
1	C	388	GLN	2.7
1	B	71	LYS	2.7
1	D	338	ASN	2.7
1	C	62	TRP	2.7
1	C	91	GLU	2.7
1	D	716	SER	2.7
1	D	141	GLN	2.7
1	D	339	CYS	2.7
1	D	655	PRO	2.7
1	C	138	ASN	2.7
1	C	391	LYS	2.7
1	A	72	GLN	2.7
1	C	140	ARG	2.7
1	C	276	LEU	2.7
1	D	703	ILE	2.7
1	C	700	TYR	2.7
1	B	676	PRO	2.7
1	D	335	GLY	2.7
1	C	277	SER	2.6
1	C	482	LEU	2.6
1	A	77	LEU	2.6
1	D	68	TYR	2.6
1	A	711	VAL	2.6
1	A	632	GLY	2.6
1	B	82	GLU	2.6
1	B	392	LYS	2.6
1	A	654	ALA	2.6
1	A	717	ALA	2.6
1	C	231	THR	2.6
1	D	365	THR	2.6
1	D	546	VAL	2.6
1	D	636	THR	2.6
1	D	95	PHE	2.6
1	A	640	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	389	ILE	2.5
1	C	100	HIS	2.5
1	A	180	LEU	2.5
1	C	393	ASP	2.5
1	D	67	GLU	2.5
1	C	637	SER	2.5
1	A	715	GLN	2.5
1	D	342	ALA	2.5
1	D	499	ALA	2.5
1	C	139	LYS	2.5
1	D	523	LYS	2.5
1	B	99	GLY	2.5
1	C	336	ARG	2.5
1	A	392	LYS	2.5
1	D	411	THR	2.5
1	A	704	HIS	2.5
1	D	54	ARG	2.5
1	D	370	SER	2.5
1	B	628	GLY	2.4
1	D	442	VAL	2.4
1	B	703	ILE	2.4
1	D	380	GLY	2.4
1	D	633	GLY	2.4
1	D	440	THR	2.4
1	A	688	VAL	2.4
1	C	537	SER	2.4
1	D	677	GLU	2.4
1	C	72	GLN	2.4
1	A	546	VAL	2.4
1	D	432	TYR	2.4
1	B	713	PHE	2.4
1	D	717	ALA	2.4
1	B	653	VAL	2.4
1	B	733	MET	2.4
1	D	733	MET	2.4
1	D	656	VAL	2.4
1	C	333	SER	2.4
1	B	702	LEU	2.4
1	D	393	ASP	2.3
1	C	711	VAL	2.3
1	B	521	GLU	2.3
1	C	452	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	636	THR	2.3
1	A	63	ILE	2.3
1	A	142	LEU	2.3
1	A	628	GLY	2.3
1	A	650	GLY	2.3
1	D	415	LEU	2.3
1	A	91	GLU	2.3
1	A	657	SER	2.3
1	C	87	SER	2.3
1	C	113	PHE	2.3
1	D	222	PHE	2.3
1	A	280	THR	2.3
1	B	241	TYR	2.3
1	D	70	TYR	2.3
1	D	704	HIS	2.3
1	D	41	LYS	2.3
1	C	715	GLN	2.3
1	A	90	LEU	2.3
1	A	543	LEU	2.3
1	A	631	TYR	2.3
1	C	655	PRO	2.2
1	A	103	ASN	2.2
1	A	638	MET	2.2
1	B	577	SER	2.2
1	C	54	ARG	2.2
1	D	71	LYS	2.2
1	A	474	GLY	2.2
1	B	656	VAL	2.2
1	C	546	VAL	2.2
1	A	231	THR	2.2
1	B	544	LEU	2.2
1	C	115	LEU	2.2
1	B	633	GLY	2.2
1	C	703	ILE	2.2
1	D	346	ILE	2.2
1	B	632	GLY	2.2
1	A	71	LYS	2.2
1	D	416	TYR	2.2
1	B	79	PHE	2.2
1	D	72	GLN	2.2
1	D	388	GLN	2.2
1	A	99	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	502	LYS	2.2
1	D	75	ASN	2.2
1	A	733	MET	2.2
1	C	688	VAL	2.2
1	A	300	LEU	2.2
1	C	483	HIS	2.2
1	C	704	HIS	2.2
1	B	711	VAL	2.2
1	C	651	ILE	2.2
1	D	63	ILE	2.2
1	D	390	ASP	2.2
1	A	633	GLY	2.2
1	A	625	ALA	2.1
1	C	84	GLY	2.1
1	D	392	LYS	2.1
1	B	631	TYR	2.1
1	D	735	TYR	2.1
1	C	76	ILE	2.1
1	D	384	ILE	2.1
1	D	79	PHE	2.1
1	D	484	SER	2.1
1	A	506	ASN	2.1
1	C	338	ASN	2.1
1	C	521	GLU	2.1
1	A	299	TYR	2.1
1	C	341	VAL	2.1
1	A	214	LEU	2.1
1	C	89	PHE	2.1
1	D	276	LEU	2.1
1	D	336	ARG	2.1
1	D	500	LEU	2.1
1	D	684	ARG	2.1
1	C	635	VAL	2.1
1	D	653	VAL	2.1
1	A	66	HIS	2.1
1	A	316	LEU	2.1
1	B	704	HIS	2.1
1	C	101	SER	2.1
1	A	78	VAL	2.1
1	C	468	TYR	2.1
1	C	491	LEU	2.1
1	D	410	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	360	SER	2.0
1	A	467	TYR	2.0
1	B	76	ILE	2.0
1	C	90	LEU	2.0
1	D	391	LYS	2.0
1	D	736	THR	2.0
1	B	333	SER	2.0
1	C	278	SER	2.0
1	C	63	ILE	2.0
1	D	348	MET	2.0
1	A	358[A]	ARG	2.0
1	D	87	SER	2.0
1	D	82	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	808	14/15	0.86	0.30	3.93	61,63,64,64	0
2	NAG	C	802	14/15	0.88	0.32	3.74	68,70,74,74	0
2	NAG	B	804	14/15	0.87	0.22	1.74	67,69,73,77	0
3	B2Y	B	800	14/14	0.88	0.28	1.20	60,62,63,64	0
3	B2Y	C	800	14/14	0.89	0.25	0.62	50,54,55,55	0
2	NAG	A	804	14/15	0.94	0.21	0.31	58,60,62,66	0
2	NAG	A	801	14/15	0.64	0.32	0.23	72,73,74,74	0
3	B2Y	A	800	14/14	0.88	0.24	0.10	53,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	C	803	14/15	0.90	0.19	-0.05	63,65,68,72	0
3	B2Y	D	800	14/14	0.93	0.17	-0.10	42,44,46,46	0
2	NAG	D	802	14/15	0.92	0.16	-0.85	55,58,61,63	0
2	NAG	B	802	14/15	0.89	0.20	-	63,64,66,66	0
2	NAG	B	806	14/15	0.80	0.14	-	67,69,73,74	0
2	NAG	A	806	14/15	0.76	0.24	-	73,76,79,80	0
2	NAG	A	807	14/15	0.82	0.35	-	83,84,85,85	0
2	NAG	D	804	14/15	0.82	0.20	-	78,80,82,82	0
2	NAG	B	805	14/15	0.82	0.43	-	80,82,83,83	0
2	NAG	C	804	14/15	0.81	0.34	-	73,76,78,78	0
2	NAG	A	803	14/15	0.72	0.33	-	71,73,76,77	0
2	NAG	B	801	14/15	0.73	0.23	-	78,79,80,80	0
2	NAG	A	802	14/15	0.77	0.30	-	65,66,68,68	0
2	NAG	A	805	14/15	0.89	0.30	-	68,70,71,71	0
2	NAG	C	801	14/15	0.77	0.20	-	55,55,56,57	0
2	NAG	D	803	14/15	0.83	0.26	-	67,68,72,72	0
2	NAG	B	803	14/15	0.81	0.33	-	63,65,68,68	0
2	NAG	D	801	14/15	0.86	0.19	-	58,60,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.