



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 07:05 PM EDT

PDB ID : 5KBY
Title : Crystal structure of dipeptidyl peptidase IV in complex with SYR-472
Authors : Skene, R.J.; Jennings, A.J.
Deposited on : 2016-06-03
Resolution : 2.24 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

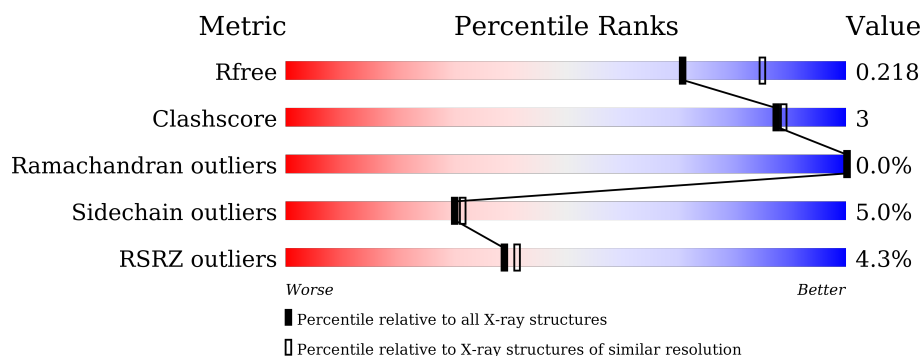
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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>4%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	B	740	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	C	740	<div> <div>7%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	D	740	<div> <div>4%</div> <div>87%</div> <div>10%</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	1504	-	-	-	X
2	NAG	A	1508	-	-	-	X
2	NAG	B	806	-	-	-	X
2	NAG	C	1505	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25867 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	725	Total	C	N	O	S	0	1	0
			5936	3813	975	1122	26			
1	B	733	Total	C	N	O	S	0	3	0
			6024	3863	1000	1135	26			
1	C	717	Total	C	N	O	S	0	2	0
			5882	3784	963	1109	26			
1	D	725	Total	C	N	O	S	0	1	0
			5946	3819	980	1121	26			

There are 48 discrepancies between the modelled and reference sequences:

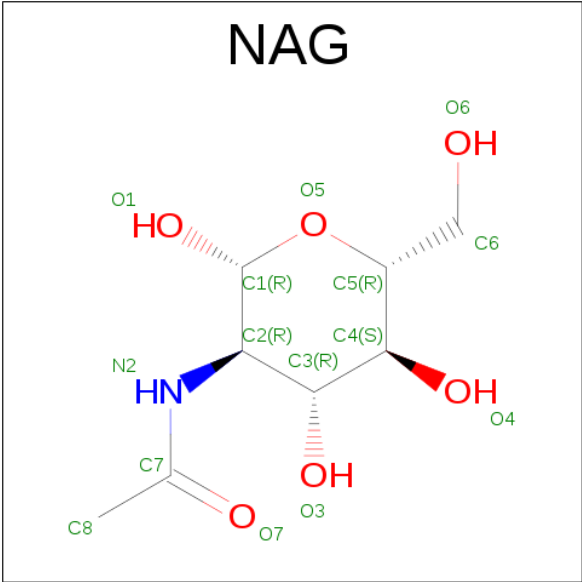
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487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



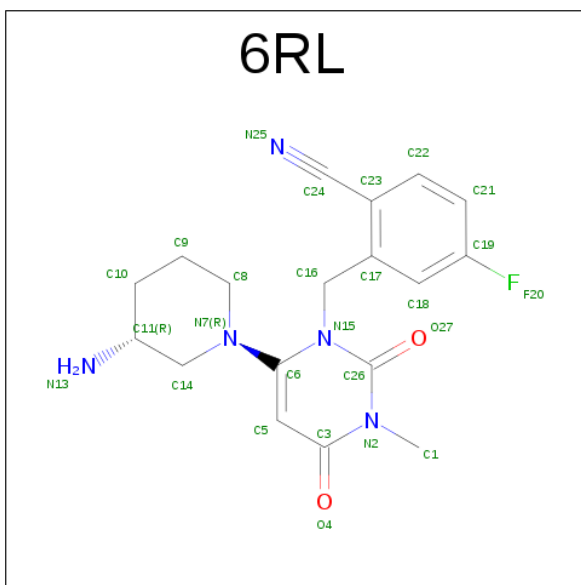
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1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

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

- Molecule 3 is 2-[[6-[(3 {R})-3-azanylpiperidin-1-yl]-3-methyl-2,4-bis(oxidanylidene)pyrimidin-1-yl]methyl]-4-fluoranyl-benzenecarbonitrile (three-letter code: 6RL) (formula: C₁₈H₂₀FN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			26	18	1	5	2		
3	B	1	Total	C	F	N	O	0	0
			26	18	1	5	2		
3	C	1	Total	C	F	N	O	0	0
			26	18	1	5	2		
3	D	1	Total	C	F	N	O	0	0
			26	18	1	5	2		

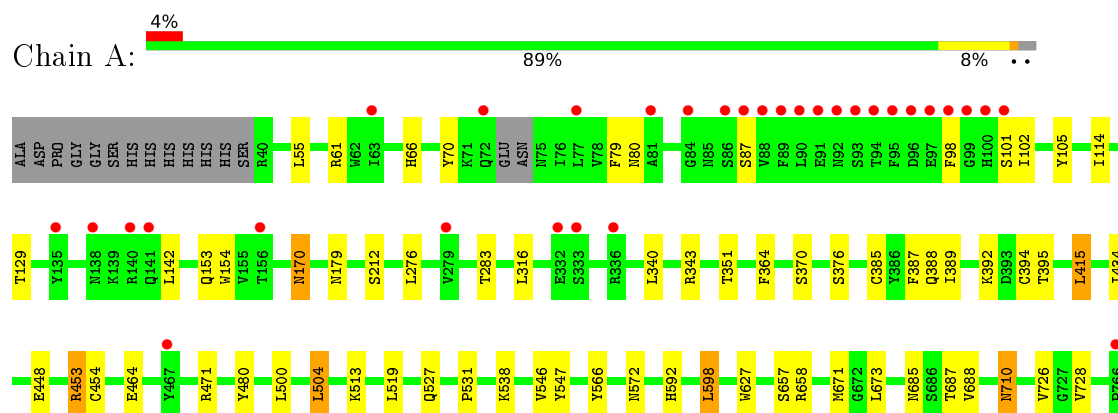
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	422	Total	O	0	0
			422	422		
4	B	497	Total	O	0	0
			497	497		
4	C	300	Total	O	0	0
			300	300		
4	D	378	Total	O	0	0
			378	378		

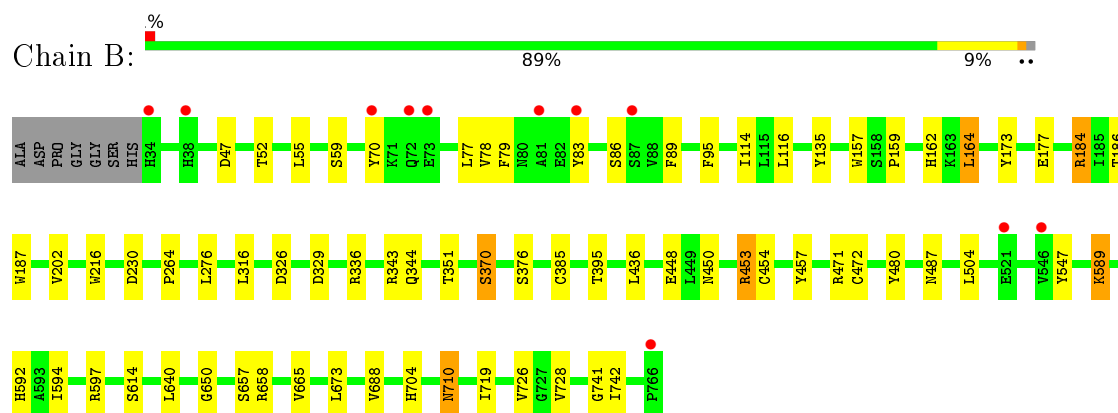
3 Residue-property plots

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

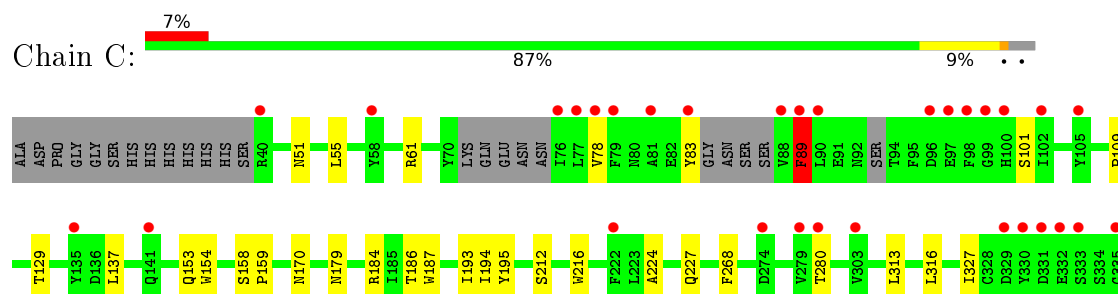
• Molecule 1: Dipeptidyl peptidase 4

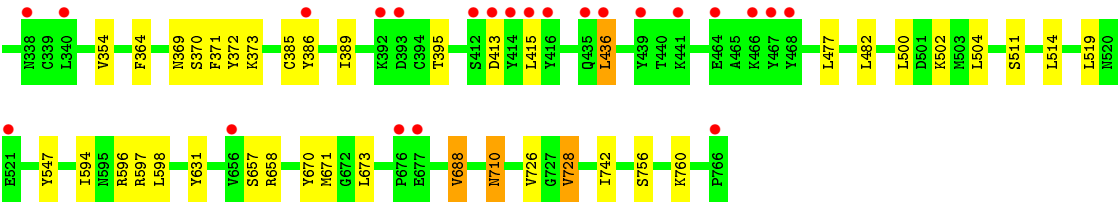


• Molecule 1: Dipeptidyl peptidase 4

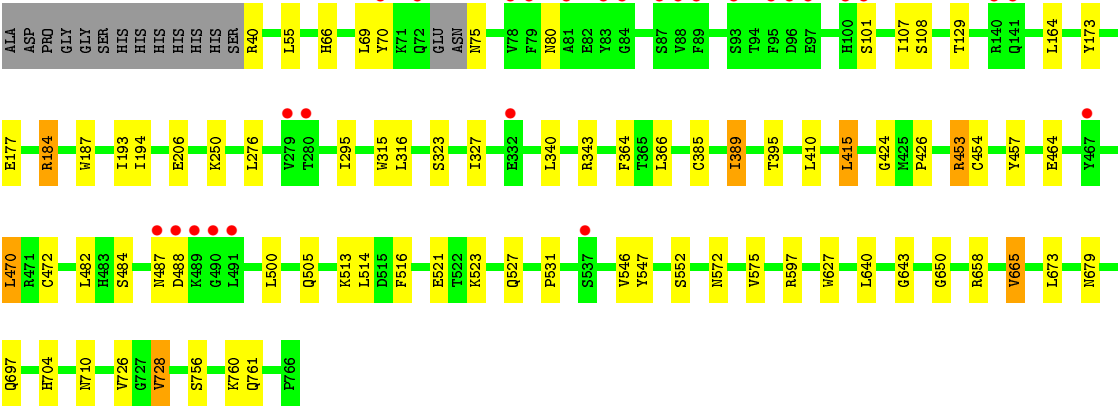
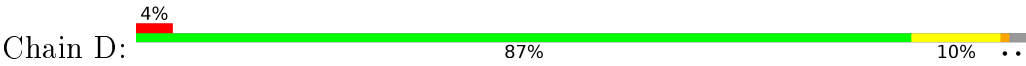


• Molecule 1: Dipeptidyl peptidase 4





● Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.57Å 122.17Å 143.70Å 90.00° 114.57° 90.00°	Depositor
Resolution (Å)	34.57 – 2.24 34.33 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.57-2.24) 97.8 (34.33-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.215 0.180 , 0.218	Depositor DCC
R_{free} test set	8950 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25867	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 6RL

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	0.42	0/6111	0.62	1/8311 (0.0%)
1	B	0.43	0/6213	0.64	1/8449 (0.0%)
1	C	0.39	0/6059	0.59	0/8239
1	D	0.40	0/6120	0.61	1/8319 (0.0%)
All	All	0.41	0/24503	0.62	3/33318 (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	B	453	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	D	415	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	453	ARG	NE-CZ-NH2	5.09	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5936	0	5651	28	0
1	B	6024	0	5725	37	0
1	C	5882	0	5600	27	0
1	D	5946	0	5669	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	126	0	114	1	0
2	B	98	0	90	0	0
2	C	70	0	63	2	0
2	D	84	0	77	1	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
4	A	422	0	0	1	0
4	B	497	0	0	4	0
4	C	300	0	0	1	0
4	D	378	0	0	1	0
All	All	25867	0	22989	123	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 3.

All (123) 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	1.30	0.79
1:C:153:GLN:HE22	1:C:170:ASN:H	1.31	0.77
1:C:369:ASN:O	1:C:389:ILE:HG12	1.86	0.75
1:D:552:SER:OG	4:D:1601:HOH:O	2.03	0.75
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.24	0.72
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.70	0.71
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.72	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.29	0.68
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.76	0.67
2:C:1503:NAG:O4	4:C:1601:HOH:O	2.15	0.65
1:C:184:ARG:HD3	1:C:186:THR:O	1.96	0.65
1:B:70:TYR:HB3	1:B:79:PHE:CE2	2.32	0.64
1:D:173:TYR:CE1	1:D:184:ARG:HG2	2.34	0.62
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.36	0.61
1:A:212[B]:SER:OG	4:A:1601:HOH:O	2.17	0.57
1:B:184:ARG:HD3	1:B:186:THR:O	2.05	0.56
1:B:657:SER:HA	1:B:688:VAL:HG13	1.89	0.55
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.71	0.54
1:B:589:LYS:HD3	4:B:947:HOH:O	2.07	0.54
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.73	0.54
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.89	0.53
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.90	0.53
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.44	0.52
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.91	0.52
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.49	0.52
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.75	0.51
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.93	0.51
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.93	0.51
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.92	0.51
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.51	0.51
1:C:78:VAL:CG2	1:C:89:PHE:HB2	2.41	0.51
1:C:194:ILE:HG12	2:C:1502:NAG:H82	1.93	0.50
1:D:107:ILE:HG22	1:D:108:SER:O	2.10	0.50
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.93	0.50
1:C:756:SER:O	1:C:760:LYS:HG3	2.11	0.50
1:D:364:PHE:HE2	1:D:389:ILE:HD11	1.77	0.50
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.92	0.50
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.94	0.50
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.93	0.50
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.95	0.49
1:D:69:LEU:C	1:D:70:TYR:CA	2.81	0.49
1:C:657:SER:HA	1:C:688:VAL:HG13	1.94	0.48
1:A:170:ASN:N	1:A:170:ASN:HD22	2.11	0.48
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.49	0.48
1:C:109:PRO:HG2	1:C:158:SER:O	2.15	0.47
1:C:742:ILE:HG22	1:C:742:ILE:O	2.13	0.47
1:D:327:ILE:HD13	1:D:389:ILE:HG13	1.95	0.47
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.49	0.47
1:D:55:LEU:HD12	1:D:500:LEU:CD2	2.44	0.47
1:B:710:ASN:C	1:B:710:ASN:HD22	2.17	0.47
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.45	0.46
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.79	0.46
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.30	0.46
1:D:726:VAL:HG23	1:D:728:VAL:CG1	2.46	0.46
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.51	0.45
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.47	0.45
1:C:372:TYR:CE1	1:C:386:TYR:CD2	3.05	0.45
1:A:351:THR:OG1	1:A:592:HIS:HD2	2.00	0.45
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.51	0.44
1:D:194:ILE:HG12	2:D:1503:NAG:H82	1.98	0.44
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.98	0.44
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.47	0.44
1:D:756:SER:O	1:D:760:LYS:HG3	2.17	0.44
1:B:370:SER:HB2	4:B:927:HOH:O	2.17	0.44
1:D:546:VAL:HG12	1:D:627:TRP:O	2.17	0.44
1:B:70:TYR:HB3	1:B:79:PHE:HE2	1.76	0.44
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.47	0.44
1:B:326:ASP:OD2	1:B:344:GLN:HG2	2.17	0.44
1:B:592:HIS:CE1	4:B:929:HOH:O	2.70	0.44
1:C:364:PHE:CD2	1:C:371:PHE:HB3	2.53	0.44
1:C:710:ASN:C	1:C:710:ASN:HD22	2.20	0.44
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.00	0.43
1:B:471[A]:ARG:HG3	1:B:480:TYR:CE1	2.53	0.43
1:A:598:LEU:HB2	1:A:671:MET:SD	2.58	0.43
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.43
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.43
1:B:592:HIS:HE1	4:B:929:HOH:O	2.01	0.43
1:B:47:ASP:HA	1:B:52:THR:OG1	2.19	0.43
1:D:516:PHE:CZ	1:D:523:LYS:HE3	2.54	0.43
1:A:657:SER:HA	1:A:688:VAL:HG13	2.01	0.42
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.82	0.42
1:D:453:ARG:HG3	1:D:454:CYS:SG	2.59	0.42
1:D:484:SER:O	1:D:488:ASP:HA	2.18	0.42
1:A:500:LEU:HG	1:A:504:LEU:HD22	2.02	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:D:173:TYR:CE1	1:D:184:ARG:CG	3.02	0.42
1:A:546:VAL:HG12	1:A:627:TRP:O	2.19	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.54	0.42
1:D:640:LEU:HD11	1:D:650:GLY:HA3	2.02	0.42
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.50	0.42
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.52	0.41
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.02	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.02	0.41
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.02	0.41
1:D:513:LYS:O	1:D:527:GLN:HA	2.21	0.41
1:B:726:VAL:HG23	1:B:728:VAL:CG1	2.50	0.41
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.50	0.41
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.36	0.41
1:B:162:HIS:NE2	1:B:177:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:CD1	1:B:86:SER:HB3	2.56	0.41
1:A:598:LEU:HD22	1:A:671:MET:CG	2.49	0.41
1:A:98:PHE:CD1	1:A:102:ILE:HD11	2.56	0.41
1:C:598:LEU:HG	1:C:631:TYR:OH	2.21	0.41
1:A:387:PHE:CD1	1:A:394:CYS:HB3	2.56	0.41
1:B:688:VAL:HG22	1:B:719:ILE:HG12	2.03	0.41
1:D:424:GLY:O	1:D:426:PRO:HD3	2.21	0.41
1:A:87:SER:H	2:A:1509:NAG:H81	1.87	0.40
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.56	0.40
1:B:471[A]:ARG:CG	1:B:480:TYR:CE1	3.04	0.40
1:D:315:TRP:O	1:D:323:SER:HB2	2.21	0.40
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.54	0.40
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.56	0.40
1:C:415:LEU:HB2	1:C:436:LEU:HD11	2.02	0.40
1:C:195:TYR:O	1:C:227:GLN:HA	2.21	0.40
1:C:596:ARG:N	1:C:670:TYR:O	2.48	0.40
1:D:457:TYR:CD1	1:D:470:LEU:HG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/740 (98%)	691 (96%)	31 (4%)	0	100	100
1	B	734/740 (99%)	711 (97%)	23 (3%)	0	100	100
1	C	711/740 (96%)	682 (96%)	28 (4%)	1 (0%)	56	65
1	D	720/740 (97%)	691 (96%)	29 (4%)	0	100	100
All	All	2887/2960 (98%)	2775 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	PHE

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%)	620 (95%)	30 (5%)	33	36
1	B	661/662 (100%)	630 (95%)	31 (5%)	32	35
1	C	644/662 (97%)	611 (95%)	33 (5%)	29	30
1	D	650/662 (98%)	613 (94%)	37 (6%)	25	25
All	All	2605/2648 (98%)	2474 (95%)	131 (5%)	30	31

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	66	HIS
1	A	80	ASN
1	A	101	SER
1	A	129	THR
1	A	142	LEU
1	A	170	ASN
1	A	179	ASN
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	340	LEU
1	A	370	SER
1	A	376	SER
1	A	385	CYS
1	A	388	GLN
1	A	392	LYS
1	A	395	THR
1	A	415	LEU
1	A	448	GLU
1	A	464	GLU

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Mol	Chain	Res	Type
1	A	504	LEU
1	A	519	LEU
1	A	538	LYS
1	A	547	TYR
1	A	566	TYR
1	A	598	LEU
1	A	673	LEU
1	A	685	ASN
1	A	710	ASN
1	B	55	LEU
1	B	59[A]	SER
1	B	59[B]	SER
1	B	77	LEU
1	B	83	TYR
1	B	164	LEU
1	B	184	ARG
1	B	202	VAL
1	B	276	LEU
1	B	316	LEU
1	B	336	ARG
1	B	370	SER
1	B	376	SER
1	B	385	CYS
1	B	395	THR
1	B	436	LEU
1	B	448	GLU
1	B	450	ASN
1	B	472	CYS
1	B	487	ASN
1	B	504	LEU
1	B	547	TYR
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	614	SER
1	B	658	ARG
1	B	665	VAL
1	B	673	LEU
1	B	704	HIS
1	B	710	ASN
1	C	51	ASN
1	C	61	ARG

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Mol	Chain	Res	Type
1	C	83	TYR
1	C	89	PHE
1	C	101	SER
1	C	129	THR
1	C	137	LEU
1	C	179	ASN
1	C	280	THR
1	C	313	LEU
1	C	316	LEU
1	C	354	VAL
1	C	370	SER
1	C	373	LYS
1	C	385	CYS
1	C	395	THR
1	C	413	ASP
1	C	436	LEU
1	C	477	LEU
1	C	482	LEU
1	C	502	LYS
1	C	504	LEU
1	C	511	SER
1	C	514	LEU
1	C	519	LEU
1	C	547	TYR
1	C	594	ILE
1	C	597	ARG
1	C	658	ARG
1	C	673	LEU
1	C	688	VAL
1	C	710	ASN
1	C	728	VAL
1	D	40	ARG
1	D	66	HIS
1	D	75	ASN
1	D	80	ASN
1	D	101	SER
1	D	129	THR
1	D	164	LEU
1	D	177	GLU
1	D	184	ARG
1	D	250	LYS
1	D	276	LEU

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Mol	Chain	Res	Type
1	D	295	ILE
1	D	316	LEU
1	D	366	LEU
1	D	385	CYS
1	D	389	ILE
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	453	ARG
1	D	464	GLU
1	D	470	LEU
1	D	472	CYS
1	D	482	LEU
1	D	487	ASN
1	D	505	GLN
1	D	514	LEU
1	D	521	GLU
1	D	547	TYR
1	D	575	VAL
1	D	658	ARG
1	D	665	VAL
1	D	673	LEU
1	D	704	HIS
1	D	710	ASN
1	D	728	VAL
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	153	GLN
1	A	170	ASN
1	A	455	GLN
1	A	520	ASN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	B	80	ASN
1	B	100	HIS
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	196	ASN
1	B	344	GLN
1	B	592	HIS
1	B	710	ASN
1	B	731	GLN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	506	ASN
1	C	572	ASN
1	C	592	HIS
1	C	710	ASN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	344	GLN
1	D	520	ASN
1	D	572	ASN
1	D	685	ASN
1	D	697	GLN
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 ⓘ

31 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	NAG	A	1501	1,2	14,14,15	0.64	0	15,19,21	1.69	4 (26%)
2	NAG	A	1502	2	14,14,15	0.47	0	15,19,21	0.92	0
2	NAG	A	1503	1	14,14,15	0.67	0	15,19,21	1.56	4 (26%)
2	NAG	A	1504	1,2	14,14,15	0.64	0	15,19,21	0.86	0
2	NAG	A	1505	2	14,14,15	0.38	0	15,19,21	1.54	3 (20%)
2	NAG	A	1506	1,2	14,14,15	0.46	0	15,19,21	0.94	1 (6%)
2	NAG	A	1507	2	14,14,15	0.46	0	15,19,21	1.31	2 (13%)
2	NAG	A	1508	1	14,14,15	0.47	0	15,19,21	0.95	1 (6%)
2	NAG	A	1509	1	14,14,15	0.58	0	15,19,21	1.13	1 (6%)
3	6RL	A	1510	-	23,28,28	0.89	0	25,40,40	1.34	4 (16%)
2	NAG	B	801	1	14,14,15	0.50	0	15,19,21	2.01	4 (26%)
2	NAG	B	802	1	14,14,15	0.44	0	15,19,21	2.70	4 (26%)
2	NAG	B	803	1,2	14,14,15	0.57	0	15,19,21	1.04	1 (6%)
2	NAG	B	804	2	14,14,15	0.49	0	15,19,21	1.37	2 (13%)
2	NAG	B	805	1	14,14,15	0.34	0	15,19,21	1.42	2 (13%)
2	NAG	B	806	1	14,14,15	0.52	0	15,19,21	1.37	2 (13%)
2	NAG	B	807	1	14,14,15	0.53	0	15,19,21	0.80	0
3	6RL	B	808	-	23,28,28	0.81	0	25,40,40	1.47	5 (20%)
2	NAG	C	1501	1	14,14,15	0.54	0	15,19,21	1.60	3 (20%)
2	NAG	C	1502	1,2	14,14,15	0.69	0	15,19,21	1.19	2 (13%)
2	NAG	C	1503	2	14,14,15	0.56	0	15,19,21	1.58	4 (26%)
2	NAG	C	1504	1	14,14,15	0.47	0	15,19,21	1.24	1 (6%)
2	NAG	C	1505	1	14,14,15	0.79	0	15,19,21	1.71	2 (13%)
3	6RL	C	1506	-	23,28,28	0.87	0	25,40,40	1.30	2 (8%)
2	NAG	D	1501	1	14,14,15	0.55	0	15,19,21	1.77	2 (13%)
2	NAG	D	1502	1	14,14,15	0.62	0	15,19,21	0.99	1 (6%)
2	NAG	D	1503	1,2	14,14,15	0.70	0	15,19,21	1.01	0
2	NAG	D	1504	2	14,14,15	0.45	0	15,19,21	1.32	2 (13%)
2	NAG	D	1505	1	14,14,15	0.54	0	15,19,21	0.88	0
2	NAG	D	1506	1	14,14,15	0.60	0	15,19,21	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6RL	D	1507	-	23,28,28	0.81	0	25,40,40	1.39	6 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1502	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1505	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1507	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1509	1	-	0/6/23/26	0/1/1/1
3	6RL	A	1510	-	-	0/10/20/20	0/3/3/3
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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	804	2	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	0/6/23/26	0/1/1/1
3	6RL	B	808	-	-	0/10/20/20	0/3/3/3
2	NAG	C	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1503	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1505	1	-	0/6/23/26	0/1/1/1
3	6RL	C	1506	-	-	0/10/20/20	0/3/3/3
2	NAG	D	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1502	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1503	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1504	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1505	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1506	1	-	0/6/23/26	0/1/1/1
3	6RL	D	1507	-	-	0/10/20/20	0/3/3/3

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	NAG	C4-C3-C2	-3.94	105.23	111.34
2	A	1501	NAG	C4-C3-C2	-3.41	106.05	111.34
2	A	1507	NAG	C4-C3-C2	-3.11	106.52	111.34
3	B	808	6RL	C10-C9-C8	-3.07	106.75	110.94
2	B	801	NAG	O7-C7-C8	-2.88	116.78	122.07
2	D	1501	NAG	C4-C3-C2	-2.64	107.25	111.34
2	C	1503	NAG	O7-C7-C8	-2.61	117.27	122.07
2	B	801	NAG	C4-C3-C2	-2.50	107.46	111.34
2	C	1503	NAG	C4-C3-C2	-2.45	107.54	111.34
2	A	1506	NAG	O4-C4-C3	-2.40	104.95	110.36
2	C	1502	NAG	O4-C4-C3	-2.34	105.08	110.36
3	C	1506	6RL	C21-C19-C18	-2.32	120.38	123.32
3	D	1507	6RL	C16-C17-C18	-2.31	115.84	119.52
3	B	808	6RL	C16-C17-C18	-2.28	115.89	119.52
3	A	1510	6RL	C10-C9-C8	-2.28	107.84	110.94
2	A	1505	NAG	O7-C7-C8	-2.27	117.89	122.07
2	A	1503	NAG	O3-C3-C4	-2.20	105.39	110.36
2	C	1501	NAG	O7-C7-C8	-2.17	118.07	122.07
3	D	1507	6RL	C21-C22-C23	-2.16	118.45	120.81
2	D	1502	NAG	O7-C7-C8	-2.15	118.12	122.07
2	A	1503	NAG	O6-C6-C5	-2.14	104.15	111.30
2	A	1503	NAG	O7-C7-C8	-2.09	118.22	122.07
3	A	1510	6RL	C9-C10-C11	-2.06	109.13	111.97
2	A	1503	NAG	C3-C4-C5	-2.05	106.57	110.23
2	B	806	NAG	O7-C7-C8	-2.02	118.36	122.07
3	D	1507	6RL	C18-C17-C23	2.02	120.21	117.81
2	B	803	NAG	C1-O5-C5	2.08	115.20	112.14
3	B	808	6RL	C10-C11-C14	2.09	112.54	109.71
2	B	804	NAG	C2-N2-C7	2.12	125.86	123.11
2	B	802	NAG	C3-C4-C5	2.13	114.03	110.23
3	D	1507	6RL	C17-C23-C24	2.14	122.04	120.14
2	C	1502	NAG	C1-O5-C5	2.14	115.29	112.14
2	B	805	NAG	O5-C5-C6	2.14	111.93	107.34
3	B	808	6RL	C17-C23-C24	2.15	122.04	120.14
2	A	1501	NAG	O3-C3-C2	2.16	114.00	109.37
3	A	1510	6RL	C16-C17-C23	2.23	123.38	120.36
2	A	1507	NAG	O3-C3-C2	2.24	114.16	109.37
2	A	1508	NAG	C1-O5-C5	2.27	115.47	112.14
2	C	1505	NAG	C3-C4-C5	2.33	114.38	110.23
2	C	1503	NAG	C1-O5-C5	2.34	115.58	112.14
3	C	1506	6RL	C17-C23-C24	2.40	122.26	120.14
2	A	1501	NAG	C2-N2-C7	2.47	126.32	123.11
2	A	1505	NAG	C2-N2-C7	2.48	126.33	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1506	NAG	C4-C3-C2	2.50	115.21	111.34
2	A	1501	NAG	C1-O5-C5	2.51	115.83	112.14
2	D	1504	NAG	C2-N2-C7	2.54	126.41	123.11
3	D	1507	6RL	C16-N15-C26	2.65	121.04	117.97
3	D	1507	6RL	C16-C17-C23	2.65	123.95	120.36
2	C	1501	NAG	C8-C7-N2	2.94	121.74	116.10
2	D	1504	NAG	C8-C7-N2	3.01	121.86	116.10
2	A	1509	NAG	C1-O5-C5	3.05	116.62	112.14
2	B	801	NAG	C8-C7-N2	3.05	121.94	116.10
2	D	1506	NAG	C1-O5-C5	3.08	116.67	112.14
2	B	804	NAG	C8-C7-N2	3.21	122.25	116.10
2	A	1505	NAG	C8-C7-N2	3.36	122.55	116.10
2	C	1503	NAG	C8-C7-N2	3.42	122.65	116.10
3	A	1510	6RL	C17-C23-C24	3.44	123.18	120.14
3	B	808	6RL	C16-C17-C23	3.53	125.13	120.36
2	B	805	NAG	C1-O5-C5	3.61	117.45	112.14
2	C	1504	NAG	C1-O5-C5	3.91	117.88	112.14
2	B	806	NAG	C1-O5-C5	3.96	117.96	112.14
2	C	1501	NAG	C1-O5-C5	4.08	118.15	112.14
2	B	802	NAG	O5-C5-C4	4.40	117.42	110.13
2	C	1505	NAG	C4-C3-C2	5.13	119.30	111.34
2	D	1501	NAG	C1-O5-C5	5.19	119.77	112.14
2	B	801	NAG	C1-O5-C5	5.36	120.03	112.14
2	B	802	NAG	C1-O5-C5	7.80	123.62	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1509	NAG	1	0
2	C	1502	NAG	1	0
2	C	1503	NAG	1	0
2	D	1503	NAG	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, 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	725/740 (97%)	0.03	32 (4%) 38 40	23, 43, 88, 137	0
1	B	733/740 (99%)	-0.23	11 (1%) 76 78	23, 42, 74, 108	0
1	C	717/740 (96%)	0.19	54 (7%) 17 18	24, 55, 102, 135	0
1	D	725/740 (97%)	0.04	28 (3%) 43 45	22, 48, 94, 124	0
All	All	2900/2960 (97%)	0.01	125 (4%) 39 41	22, 46, 92, 137	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	GLU	7.4
1	D	81	ALA	6.2
1	A	81	ALA	6.0
1	C	77	LEU	6.0
1	C	335	GLY	5.6
1	A	86	SER	5.5
1	A	96	ASP	5.3
1	D	89	PHE	5.2
1	D	84	GLY	5.2
1	D	83	TYR	4.9
1	A	88	VAL	4.8
1	C	439	TYR	4.7
1	A	89	PHE	4.7
1	C	89	PHE	4.7
1	D	279	VAL	4.6
1	A	97	GLU	4.4
1	C	88	VAL	4.4
1	D	487	ASN	4.4
1	D	70	TYR	4.3
1	A	98	PHE	4.3
1	C	76	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	392	LYS	4.3
1	B	83	TYR	4.3
1	C	330	TYR	4.1
1	B	87	SER	4.1
1	D	87	SER	4.1
1	C	96	ASP	4.1
1	C	99	GLY	4.1
1	A	93	SER	4.1
1	C	766	PRO	4.0
1	A	279	VAL	4.0
1	A	90	LEU	4.0
1	B	70	TYR	3.9
1	A	99	GLY	3.9
1	C	81	ALA	3.9
1	C	100	HIS	3.7
1	C	412	SER	3.7
1	D	490	GLY	3.7
1	A	72	GLN	3.7
1	A	87	SER	3.6
1	A	140	ARG	3.6
1	C	333	SER	3.6
1	B	73	GLU	3.5
1	C	78	VAL	3.4
1	A	95	PHE	3.4
1	D	93	SER	3.4
1	A	332	GLU	3.3
1	C	332	GLU	3.3
1	D	78	VAL	3.3
1	C	98	PHE	3.3
1	D	489	LYS	3.2
1	C	464	GLU	3.2
1	D	79	PHE	3.1
1	A	92	ASN	3.1
1	C	331	ASP	3.0
1	C	414	TYR	3.0
1	D	537	SER	3.0
1	B	521	GLU	3.0
1	C	415	LEU	3.0
1	D	96	ASP	3.0
1	B	34	HIS	3.0
1	A	138	ASN	3.0
1	D	141	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	83	TYR	2.9
1	D	95	PHE	2.9
1	A	77	LEU	2.9
1	D	140	ARG	2.8
1	D	280	THR	2.8
1	D	491	LEU	2.8
1	A	766	PRO	2.8
1	C	105	TYR	2.8
1	A	467	TYR	2.7
1	C	274	ASP	2.7
1	C	413	ASP	2.6
1	B	72	GLN	2.6
1	B	766	PRO	2.6
1	A	141	GLN	2.6
1	C	40	ARG	2.6
1	A	333	SER	2.5
1	C	79	PHE	2.5
1	A	135	TYR	2.5
1	C	656	VAL	2.4
1	C	467	TYR	2.4
1	D	100	HIS	2.4
1	C	338	ASN	2.4
1	A	91	GLU	2.4
1	C	90	LEU	2.4
1	A	100	HIS	2.4
1	D	332	GLU	2.4
1	C	441	LYS	2.4
1	D	72	GLN	2.4
1	C	521	GLU	2.4
1	C	676	PRO	2.4
1	D	97	GLU	2.3
1	C	677	GLU	2.3
1	C	279	VAL	2.3
1	C	102	ILE	2.3
1	A	101	SER	2.3
1	C	280	THR	2.2
1	D	488	ASP	2.2
1	C	436	LEU	2.2
1	D	88	VAL	2.2
1	C	468	TYR	2.2
1	A	156	THR	2.2
1	C	58	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	TYR	2.2
1	A	84	GLY	2.2
1	B	81	ALA	2.2
1	C	435	GLN	2.2
1	C	466	LYS	2.1
1	A	63	ILE	2.1
1	C	303	VAL	2.1
1	C	386	TYR	2.1
1	C	141	GLN	2.1
1	C	393	ASP	2.1
1	C	416	TYR	2.1
1	C	340	LEU	2.0
1	B	546	VAL	2.0
1	A	336	ARG	2.0
1	B	38	HIS	2.0
1	D	467	TYR	2.0
1	D	101	SER	2.0
1	C	329	ASP	2.0
1	C	222	PHE	2.0
1	A	94	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, 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	B	806	14/15	0.79	0.36	7.02	67,76,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1508	14/15	0.89	0.21	5.45	59,69,73,79	0
2	NAG	C	1505	14/15	0.69	0.32	3.33	76,87,98,106	0
2	NAG	A	1504	14/15	0.96	0.19	2.01	40,46,58,60	0
2	NAG	D	1506	14/15	0.89	0.23	1.81	64,79,86,87	0
3	6RL	A	1510	26/26	0.97	0.15	-0.17	24,27,30,33	0
3	6RL	B	808	26/26	0.98	0.14	-0.21	19,26,31,33	0
3	6RL	D	1507	26/26	0.97	0.12	-0.32	22,28,32,37	0
2	NAG	A	1509	14/15	0.65	0.23	-0.36	99,115,122,124	0
3	6RL	C	1506	26/26	0.98	0.13	-0.48	26,30,34,36	0
2	NAG	B	801	14/15	0.73	0.19	-0.70	69,85,94,94	0
2	NAG	D	1503	14/15	0.94	0.12	-1.08	47,54,68,71	0
2	NAG	B	803	14/15	0.95	0.11	-1.31	44,54,63,74	0
2	NAG	C	1502	14/15	0.96	0.08	-1.53	37,47,54,58	0
2	NAG	B	804	14/15	0.77	0.25	-	62,85,99,105	0
2	NAG	B	802	14/15	0.86	0.21	-	56,63,67,71	0
2	NAG	C	1504	14/15	0.81	0.15	-	61,83,107,108	0
2	NAG	D	1505	14/15	0.74	0.19	-	74,84,91,96	0
2	NAG	A	1507	14/15	0.85	0.24	-	88,93,99,102	0
2	NAG	C	1501	14/15	0.71	0.17	-	64,74,83,85	0
2	NAG	A	1506	14/15	0.89	0.16	-	60,80,91,92	0
2	NAG	B	807	14/15	0.87	0.28	-	54,65,72,75	0
2	NAG	C	1503	14/15	0.93	0.17	-	50,58,67,69	0
2	NAG	B	805	14/15	0.81	0.16	-	64,71,78,79	0
2	NAG	A	1502	14/15	0.73	0.47	-	101,120,128,132	0
2	NAG	D	1504	14/15	0.82	0.36	-	60,93,108,112	0
2	NAG	A	1503	14/15	0.79	0.38	-	35,40,50,51	0
2	NAG	D	1502	14/15	0.89	0.31	-	60,68,81,85	0
2	NAG	A	1505	14/15	0.87	0.28	-	59,69,73,75	0
2	NAG	D	1501	14/15	0.82	0.24	-	66,77,88,89	0
2	NAG	A	1501	14/15	0.66	0.31	-	75,86,99,114	0

6.5 Other polymers

There are no such residues in this entry.