W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:29 PM GMT

PDB ID	:	2ZNH
Title	:	Crystal Structure of a Domain-Swapped Serpin Dimer
Authors	:	Yamasaki, M.; Huntington, J.A.
Deposited on	:	2008-04-25
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance ⓘ
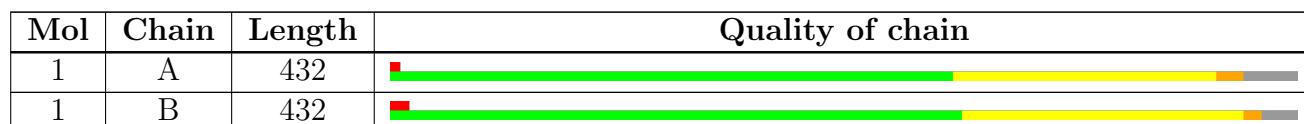
The reported resolution of this entry is 2.80 Å.

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		19
Ramachandran outliers		1.7%
Sidechain outliers		4.2%
RSRZ outliers		1.6%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	701	-	X
4	NAG	B	501	-	X
5	CIT	B	604	-	X
5	CIT	B	605	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6599 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total 3156	C 2026	N 523	O 589	S 18	0	0	0
1	B	412	Total 3192	C 2045	N 530	O 599	S 18	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total 28	C 16	N 2	O 10	0	0
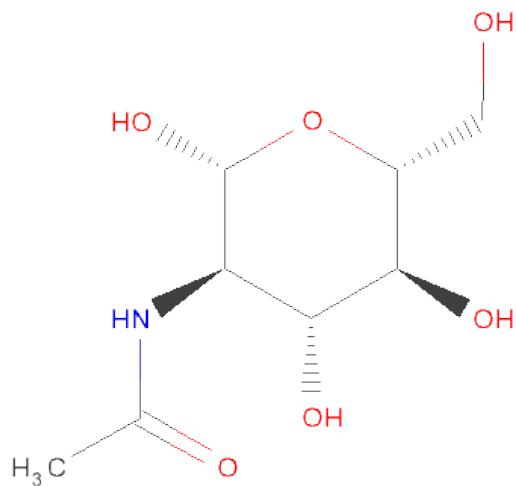
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total 39	C 22	N 2	O 15	0	0
3	B	3	Total 39	C 22	N 2	O 15	0	0
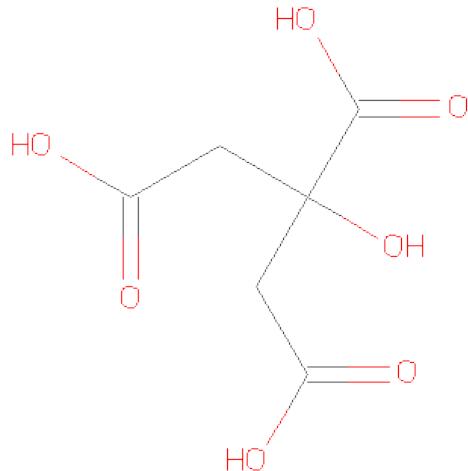
- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 13	C 6	O 7	0	0
5	B	1	Total 13	C 6	O 7	0	0

- Molecule 6 is water.
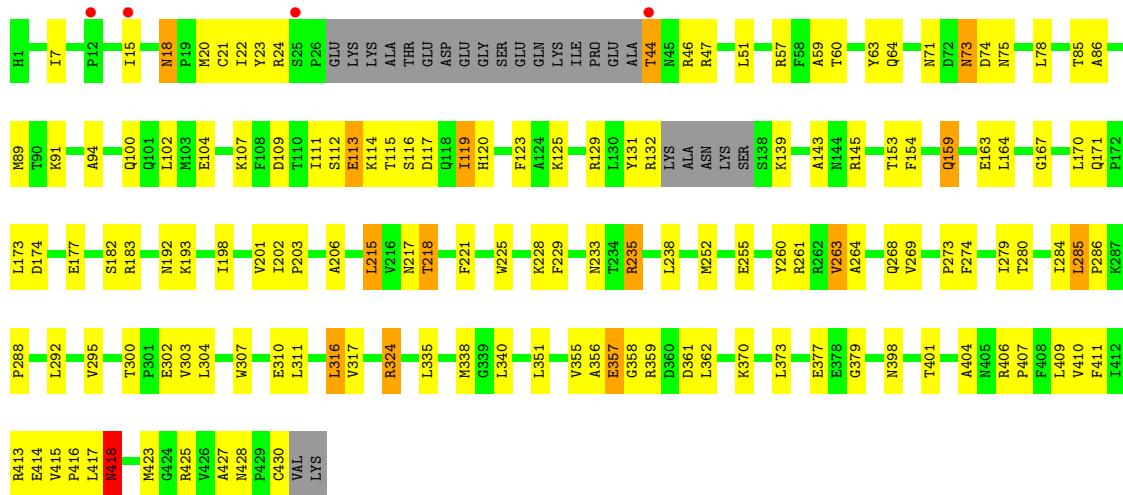
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total 36	O 36	0	0
6	B	55	Total 55	O 55	0	0

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.
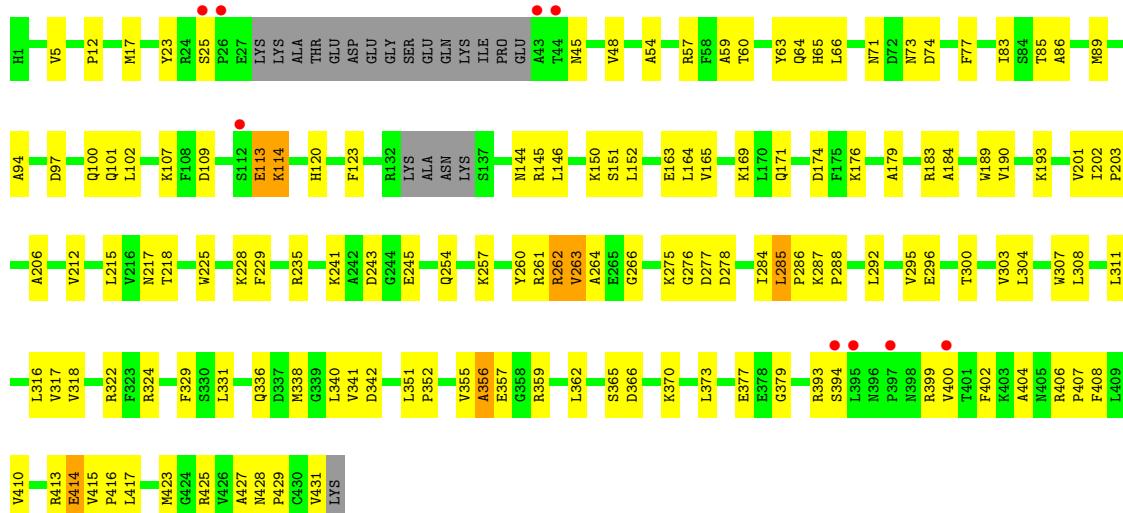
- Molecule 1: Antithrombin-III

Chain A:

- Molecule 1: Antithrombin-III

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.35Å 99.88Å 92.46Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	43.77 – 2.80 43.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.77-2.80) 99.6 (43.77-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.247 0.201 , 0.243	Depositor DCC
R_{free} test set	1603 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 31423 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.40	0/3222	0.65	1/4369 (0.0%)
1	B	0.38	0/3258	0.64	1/4417 (0.0%)
All	All	0.39	0/6480	0.64	2/8786 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	LEU	N-CA-C	-7.60	90.49	111.00
1	B	414	GLU	N-CA-C	-5.29	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3156	0	3068	124	0
1	B	3192	0	3094	130	0
2	A	28	0	25	0	0
3	A	39	0	34	2	0
3	B	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	2	0
4	B	14	0	13	0	0
5	B	26	0	11	4	0
6	A	36	0	0	1	0
6	B	55	0	0	8	0
All	All	6599	0	6292	241	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (241) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:VAL:HG12	1:B:264:ALA:H	1.04	1.09
1:A:263:VAL:HG12	1:A:264:ALA:H	1.13	1.07
1:B:393:ARG:HG2	1:B:394:SER:H	1.35	0.91
1:B:285:LEU:HD13	1:B:408:PHE:HB3	1.53	0.90
1:B:263:VAL:HG12	1:B:264:ALA:N	1.86	0.89
1:A:263:VAL:HG12	1:A:264:ALA:N	1.91	0.85
1:A:59:ALA:HB1	1:A:423:MET:HE1	1.57	0.85
1:B:57:ARG:HG2	1:B:107:LYS:HG2	1.59	0.83
1:B:65:HIS:CD2	1:B:338:MET:HG2	2.16	0.80
1:A:286:PRO:HB3	1:A:295:VAL:HG21	1.64	0.79
1:A:263:VAL:CG1	1:A:264:ALA:H	1.95	0.78
1:B:407:PRO:HB3	1:B:427:ALA:HA	1.65	0.78
1:A:143:ALA:H	1:A:218:THR:HG22	1.50	0.77
1:A:415:VAL:HG23	1:A:416:PRO:HD3	1.65	0.76
1:A:310:GLU:HA	1:A:310:GLU:OE1	1.84	0.76
1:B:393:ARG:HG2	1:B:394:SER:N	2.01	0.76
1:B:151:SER:OG	1:B:176:LYS:HE2	1.86	0.75
1:A:407:PRO:HB3	1:A:427:ALA:HA	1.69	0.75
1:B:23:TYR:CE1	1:B:100:GLN:HG3	2.22	0.74
1:B:287:LYS:HG2	1:B:288:PRO:HD2	1.68	0.74
1:A:145:ARG:NH1	1:A:171:GLN:HB2	2.05	0.72
1:A:145:ARG:HH11	1:A:171:GLN:HB2	1.55	0.71
1:A:417:LEU:C	1:A:418:ASN:HD22	1.94	0.71
1:A:15:ILE:HG23	1:A:164:LEU:HD21	1.74	0.70
1:A:414:GLU:OE1	1:A:416:PRO:HG2	1.92	0.69
1:B:263:VAL:CG1	1:B:264:ALA:H	1.89	0.69
1:A:255:GLU:HB3	1:A:317:VAL:HG22	1.75	0.69
1:A:71:ASN:HB3	1:A:74:ASP:OD2	1.93	0.69
1:B:341:VAL:HG13	1:B:342:ASP:H	1.58	0.69
1:A:193:LYS:HB3	1:A:218:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:THR:OG1	1:A:303:VAL:HG23	1.93	0.68
1:A:340:LEU:HD12	1:B:336:GLN:HB3	1.77	0.67
1:A:173:LEU:HD13	1:A:182:SER:HB3	1.75	0.67
1:B:276:GLY:O	1:B:277:ASP:HB2	1.94	0.66
1:A:201:VAL:HG13	1:A:202:ILE:HG13	1.76	0.66
1:A:24:ARG:HA	1:A:114:LYS:O	1.94	0.66
1:A:215:LEU:H	1:A:215:LEU:HD12	1.61	0.65
1:B:414:GLU:HG2	1:B:417:LEU:HB2	1.78	0.65
1:B:243:ASP:OD1	1:B:245:GLU:HG2	1.96	0.65
1:B:183:ARG:NH1	1:B:202:ILE:O	2.29	0.65
1:B:341:VAL:HG13	1:B:342:ASP:N	2.10	0.65
3:B:602:NAG:O3	3:B:603:MAN:H2	1.97	0.65
1:B:278:ASP:HB2	6:B:650:HOH:O	1.96	0.64
1:A:413:ARG:CZ	1:A:415:VAL:HG12	2.27	0.64
1:A:215:LEU:N	1:A:215:LEU:HD12	2.13	0.63
1:B:215:LEU:HD12	1:B:215:LEU:N	2.14	0.63
1:B:414:GLU:CG	1:B:417:LEU:HB2	2.28	0.63
1:B:316:LEU:C	1:B:316:LEU:HD12	2.18	0.63
3:A:601:NAG:H81	1:B:356:ALA:O	1.98	0.63
1:B:356:ALA:O	1:B:357:GLU:HG3	1.99	0.62
1:A:415:VAL:HG23	1:A:416:PRO:CD	2.30	0.61
1:A:7:ILE:HG13	1:A:15:ILE:HG13	1.82	0.61
1:A:406:ARG:HB3	1:A:407:PRO:HD2	1.82	0.61
1:B:145:ARG:NH1	1:B:171:GLN:HB2	2.16	0.61
1:B:71:ASN:ND2	1:B:73:ASN:HB2	2.17	0.60
1:A:71:ASN:ND2	1:A:73:ASN:HB2	2.17	0.60
1:B:243:ASP:O	1:B:399:ARG:HD3	2.02	0.60
1:B:59:ALA:HB1	1:B:423:MET:HE2	1.85	0.59
1:A:174:ASP:OD2	1:A:177:GLU:HB3	2.03	0.59
1:A:91:LYS:HG3	1:A:102:LEU:HD23	1.84	0.59
1:A:414:GLU:HG2	1:A:417:LEU:HB2	1.85	0.59
1:A:86:ALA:HA	1:A:89:MET:HE2	1.85	0.59
1:B:190:VAL:HG22	1:B:218:THR:CG2	2.32	0.59
1:B:83:ILE:HD13	1:B:331:LEU:HD21	1.85	0.59
1:A:23:TYR:CE1	1:A:100:GLN:HG3	2.38	0.59
1:A:85:THR:HG21	1:A:217:ASN:ND2	2.18	0.58
1:B:415:VAL:HG23	1:B:416:PRO:HD3	1.86	0.57
1:B:241:LYS:HD3	1:B:428:ASN:ND2	2.18	0.57
1:A:285:LEU:HD23	1:A:406:ARG:NH2	2.19	0.57
1:B:414:GLU:OE1	1:B:416:PRO:HG2	2.05	0.57
1:B:355:VAL:HG12	1:B:356:ALA:N	2.20	0.57
1:A:203:PRO:HG2	1:A:206:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:TYR:O	1:A:132:ARG:CB	2.53	0.56
1:A:57:ARG:HG2	1:A:107:LYS:HG3	1.88	0.56
1:A:143:ALA:N	1:A:218:THR:HG22	2.18	0.56
1:B:163:GLU:OE2	1:B:169:LYS:HG2	2.06	0.56
1:A:377:GLU:HA	1:B:229:PHE:HB2	1.88	0.55
1:A:316:LEU:HD23	1:A:316:LEU:O	2.07	0.55
1:B:355:VAL:HG23	1:B:362:LEU:HD11	1.88	0.55
1:A:159:GLN:OE1	1:A:170:LEU:HD13	2.07	0.55
1:A:273:PRO:HA	1:A:280:THR:HG22	1.89	0.54
1:B:415:VAL:CG2	1:B:416:PRO:HD3	2.38	0.54
1:A:415:VAL:CG2	1:A:416:PRO:HD3	2.36	0.54
1:A:183:ARG:HD2	1:A:203:PRO:O	2.08	0.54
1:A:377:GLU:OE1	1:B:322:ARG:NH1	2.41	0.54
1:B:152:LEU:CD2	1:B:212:VAL:HG13	2.37	0.54
1:B:201:VAL:HG13	1:B:202:ILE:HG13	1.89	0.54
1:A:418:ASN:HD22	1:A:418:ASN:N	2.06	0.53
1:B:189:TRP:CD1	5:B:605:CIT:O1	2.61	0.53
1:B:146:LEU:HD22	1:B:215:LEU:HG	1.90	0.53
1:B:400:VAL:HG13	1:B:402:PHE:CE1	2.43	0.53
4:A:701:NAG:H2	6:A:725:HOH:O	2.09	0.53
1:B:393:ARG:CG	1:B:394:SER:N	2.65	0.53
1:A:284:ILE:HD12	1:A:411:PHE:HE1	1.72	0.53
1:A:154:PHE:CD2	1:A:170:LEU:HD11	2.44	0.52
1:B:287:LYS:HG2	1:B:288:PRO:CD	2.37	0.52
1:A:85:THR:HG21	1:A:217:ASN:HD22	1.75	0.52
1:A:18:ASN:HB2	3:A:602:NAG:H81	1.90	0.52
1:A:125:LYS:O	1:A:129:ARG:HG2	2.10	0.52
1:A:229:PHE:HB2	1:B:377:GLU:HA	1.92	0.52
1:B:285:LEU:HD13	1:B:408:PHE:CB	2.34	0.52
1:A:284:ILE:HB	1:A:409:LEU:HB2	1.92	0.52
1:B:60:THR:O	1:B:64:GLN:HG3	2.10	0.52
1:B:45:ASN:HD22	1:B:48:VAL:H	1.55	0.52
1:B:286:PRO:HB3	1:B:295:VAL:HG21	1.92	0.52
1:B:23:TYR:CZ	1:B:100:GLN:HG3	2.45	0.51
1:A:192:ASN:OD1	4:A:701:NAG:N2	2.43	0.51
1:A:286:PRO:HB3	1:A:295:VAL:CG2	2.39	0.51
1:A:370:LYS:HE3	6:B:629:HOH:O	2.10	0.51
1:A:86:ALA:HA	1:A:89:MET:CE	2.40	0.51
1:B:86:ALA:HA	1:B:89:MET:CE	2.40	0.51
1:A:284:ILE:HD13	1:A:307:TRP:CZ3	2.45	0.51
1:B:404:ALA:O	1:B:406:ARG:HG2	2.11	0.51
1:B:263:VAL:HG11	1:B:307:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ARG:HD2	1:A:235:ARG:N	2.25	0.51
1:B:262:ARG:HE	1:B:266:GLY:HA2	1.76	0.51
1:B:263:VAL:CG1	1:B:264:ALA:N	2.59	0.51
1:B:284:ILE:HD13	1:B:307:TRP:CZ3	2.46	0.50
1:B:184:ALA:HA	6:B:657:HOH:O	2.11	0.50
1:A:23:TYR:HB3	1:A:116:SER:HB3	1.93	0.50
1:A:59:ALA:CB	1:A:423:MET:HE1	2.36	0.50
1:B:59:ALA:O	1:B:423:MET:HE1	2.11	0.50
1:B:150:LYS:HD3	1:B:174:ASP:HB2	1.94	0.50
1:A:102:LEU:HD12	1:B:340:LEU:HD21	1.93	0.49
1:A:351:LEU:HD23	1:B:94:ALA:HA	1.93	0.49
1:A:44:THR:OG1	1:A:44:THR:O	2.29	0.49
1:B:151:SER:HG	1:B:176:LYS:HE2	1.74	0.49
1:A:183:ARG:NH1	1:A:202:ILE:O	2.45	0.49
1:B:393:ARG:CG	1:B:394:SER:H	2.06	0.49
1:B:71:ASN:HB3	1:B:74:ASP:OD2	2.11	0.49
1:A:60:THR:O	1:A:64:GLN:HG3	2.13	0.49
1:B:308:LEU:O	1:B:311:LEU:HB2	2.13	0.49
1:A:63:TYR:OH	1:A:425:ARG:HB2	2.13	0.49
1:B:415:VAL:HG23	1:B:416:PRO:CD	2.43	0.48
1:B:415:VAL:CG2	1:B:416:PRO:CD	2.92	0.48
1:A:324:ARG:HA	1:B:373:LEU:O	2.13	0.48
1:B:97:ASP:O	1:B:101:GLN:HG3	2.13	0.48
1:A:198:ILE:HG23	1:B:370:LYS:HB3	1.95	0.48
1:A:292:LEU:HD11	1:A:409:LEU:HG	1.94	0.48
1:A:284:ILE:HD13	1:A:307:TRP:HZ3	1.78	0.48
1:A:404:ALA:O	1:A:406:ARG:NH1	2.47	0.48
1:B:85:THR:O	1:B:89:MET:HG3	2.14	0.48
1:B:17:MET:HE3	1:B:164:LEU:HD12	1.96	0.48
1:A:102:LEU:CD1	1:B:340:LEU:HD21	2.43	0.48
1:B:190:VAL:HG22	1:B:218:THR:HG21	1.96	0.47
1:B:355:VAL:CG1	1:B:356:ALA:N	2.76	0.47
1:A:91:LYS:HZ3	1:A:119:ILE:CD1	2.27	0.47
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.78	0.47
1:A:274:PHE:HD2	1:A:279:ILE:O	1.97	0.47
1:A:91:LYS:HZ1	1:A:119:ILE:HG12	1.79	0.47
1:A:22:ILE:HD12	1:A:117:ASP:OD1	2.15	0.47
1:A:410:VAL:O	1:A:423:MET:HA	2.15	0.47
1:A:233:ASN:O	1:A:235:ARG:HD2	2.15	0.47
1:A:44:THR:C	1:A:46:ARG:H	2.17	0.47
1:A:355:VAL:HG23	1:A:362:LEU:HD11	1.95	0.47
1:B:5:VAL:HG11	1:B:12:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:GLU:OE1	1:A:417:LEU:HD12	2.15	0.47
1:A:356:ALA:O	1:A:357:GLU:CB	2.62	0.47
1:B:341:VAL:HG13	1:B:342:ASP:OD1	2.15	0.46
1:B:285:LEU:N	1:B:285:LEU:HD22	2.30	0.46
1:B:193:LYS:HZ1	5:B:605:CIT:HO7	1.57	0.46
1:A:91:LYS:HE2	1:A:120:HIS:CE1	2.51	0.46
1:A:115:THR:HB	1:A:117:ASP:OD1	2.16	0.46
1:A:302:GLU:H	1:A:302:GLU:CD	2.19	0.46
1:A:21:CYS:O	1:A:22:ILE:HD13	2.16	0.46
1:B:284:ILE:HD13	1:B:307:TRP:HZ3	1.80	0.45
1:B:365:SER:O	1:B:366:ASP:HB2	2.17	0.45
1:A:414:GLU:CG	1:A:417:LEU:HB2	2.47	0.45
1:B:152:LEU:HD23	1:B:212:VAL:HG13	1.99	0.45
1:A:379:GLY:HA2	1:B:225:TRP:CD1	2.52	0.45
1:A:417:LEU:C	1:A:418:ASN:ND2	2.68	0.45
1:A:358:GLY:O	1:A:359:ARG:C	2.55	0.45
1:A:71:ASN:HD21	1:A:73:ASN:HB2	1.82	0.45
1:B:144:ASN:OD1	1:B:217:ASN:ND2	2.41	0.45
1:A:59:ALA:O	1:A:423:MET:HE3	2.17	0.44
1:B:86:ALA:HA	1:B:89:MET:HE2	1.99	0.44
1:B:300:THR:OG1	1:B:303:VAL:HG23	2.17	0.44
1:B:25:SER:OG	1:B:109:ASP:HB2	2.17	0.44
1:B:415:VAL:HG12	6:B:627:HOH:O	2.17	0.44
1:A:139:LYS:O	1:A:221:PHE:HA	2.18	0.44
1:A:417:LEU:O	1:A:418:ASN:C	2.56	0.44
1:B:54:ALA:HB1	1:B:107:LYS:O	2.17	0.44
1:A:404:ALA:O	1:A:406:ARG:HG3	2.18	0.44
1:A:335:LEU:HA	1:A:338:MET:HG3	1.98	0.44
1:A:20:MET:HG2	1:B:352:PRO:HG2	1.98	0.44
1:A:22:ILE:HG22	1:A:23:TYR:N	2.32	0.44
1:A:225:TRP:CD1	1:B:379:GLY:HA2	2.53	0.44
1:B:145:ARG:NH1	1:B:171:GLN:OE1	2.50	0.44
1:B:71:ASN:HD21	1:B:73:ASN:HB2	1.81	0.43
1:A:428:ASN:OD1	1:A:430:CYS:HB2	2.18	0.43
1:A:260:TYR:OH	1:A:268:GLN:HG2	2.19	0.43
1:B:341:VAL:CG1	1:B:342:ASP:H	2.29	0.43
1:B:316:LEU:HD11	1:B:318:VAL:HG12	1.99	0.43
1:B:189:TRP:NE1	5:B:605:CIT:O1	2.52	0.43
1:B:260:TYR:CG	1:B:261:ARG:N	2.86	0.43
1:A:111:ILE:O	1:A:113:GLU:N	2.51	0.42
1:B:406:ARG:HB3	1:B:407:PRO:HD2	2.00	0.42
1:A:415:VAL:CG2	1:A:416:PRO:CD	2.94	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:254:GLN:HG2	1:B:318:VAL:HG22	2.00	0.42
5:B:605:CIT:H41	6:B:655:HOH:O	2.18	0.42
1:B:86:ALA:HA	1:B:89:MET:HE3	2.02	0.42
1:B:292:LEU:O	1:B:296:GLU:HG3	2.19	0.42
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.93	0.42
1:B:203:PRO:HG2	1:B:206:ALA:HB2	2.01	0.42
1:B:340:LEU:HA	1:B:340:LEU:HD23	1.86	0.42
1:B:63:TYR:OH	1:B:425:ARG:HB2	2.20	0.42
1:B:341:VAL:CG1	1:B:342:ASP:N	2.80	0.41
1:A:159:GLN:HE21	1:A:159:GLN:HB2	1.58	0.41
1:A:373:LEU:HB2	1:B:77:PHE:CZ	2.55	0.41
1:A:94:ALA:HA	1:B:351:LEU:HD23	2.01	0.41
1:B:17:MET:CE	1:B:164:LEU:HD12	2.50	0.41
1:A:398:ASN:ND2	1:A:401:THR:HG22	2.35	0.41
1:B:414:GLU:HG3	1:B:417:LEU:HB2	2.03	0.41
1:B:215:LEU:CD1	1:B:215:LEU:N	2.83	0.41
1:B:113:GLU:O	1:B:114:LYS:CG	2.67	0.41
1:A:163:GLU:O	1:A:167:GLY:HA2	2.19	0.41
1:A:269:VAL:HG21	1:A:307:TRP:HB3	2.02	0.41
1:A:221:PHE:CE1	1:A:279:ILE:HG21	2.55	0.41
1:B:316:LEU:CD1	1:B:316:LEU:C	2.87	0.41
1:B:120:HIS:HB3	1:B:165:VAL:HG11	2.02	0.41
1:B:183:ARG:HD2	1:B:203:PRO:O	2.20	0.41
1:B:261:ARG:CB	1:B:311:LEU:HD12	2.50	0.41
1:A:75:ASN:OD1	1:A:427:ALA:N	2.52	0.41
1:A:229:PHE:CD2	1:A:252:MET:HB3	2.56	0.41
1:A:260:TYR:CG	1:A:261:ARG:N	2.89	0.41
1:B:413:ARG:NH2	6:B:610:HOH:O	2.54	0.41
1:B:66:LEU:HD21	1:B:329:PHE:CE2	2.55	0.41
1:A:284:ILE:HD12	1:A:411:PHE:CE1	2.53	0.41
1:B:17:MET:HE1	1:B:164:LEU:HB2	2.02	0.41
1:A:373:LEU:HB2	1:B:77:PHE:CE2	2.55	0.41
1:A:104:GLU:HA	1:A:109:ASP:OD2	2.20	0.41
1:B:410:VAL:O	1:B:423:MET:HA	2.21	0.41
1:A:316:LEU:C	1:A:316:LEU:HD23	2.41	0.41
1:A:51:LEU:HA	1:A:111:ILE:HD11	2.03	0.41
1:B:193:LYS:HB3	6:B:641:HOH:O	2.21	0.40
1:B:235:ARG:HD3	6:B:625:HOH:O	2.21	0.40
1:A:153:THR:O	1:B:356:ALA:HB2	2.21	0.40
1:B:285:LEU:N	1:B:285:LEU:CD2	2.84	0.40
1:B:261:ARG:HB3	1:B:311:LEU:HD12	2.04	0.40
1:B:254:GLN:HG2	1:B:318:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:377:GLU:OE1	1:B:377:GLU:N	2.43	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	402/432 (93%)	367 (91%)	29 (7%)	6 (2%)	15	46
1	B	406/432 (94%)	371 (91%)	27 (7%)	8 (2%)	11	35
All	All	808/864 (94%)	738 (91%)	56 (7%)	14 (2%)	14	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	VAL
1	A	112	SER
1	B	113	GLU
1	B	356	ALA
1	B	359	ARG
1	A	228	LYS
1	B	228	LYS
1	B	275	LYS
1	A	263	VAL
1	A	357	GLU
1	B	114	LYS
1	B	179	ALA
1	A	361	ASP
1	A	418	ASN

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	335/383 (88%)	317 (95%)	18 (5%)	31	66
1	B	338/383 (88%)	328 (97%)	10 (3%)	53	87
All	All	673/766 (88%)	645 (96%)	28 (4%)	40	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	44	THR
1	A	73	ASN
1	A	78	LEU
1	A	113	GLU
1	A	119	ILE
1	A	123	PHE
1	A	159	GLN
1	A	215	LEU
1	A	218	THR
1	A	235	ARG
1	A	238	LEU
1	A	285	LEU
1	A	288	PRO
1	A	304	LEU
1	A	316	LEU
1	A	324	ARG
1	A	418	ASN
1	B	102	LEU
1	B	123	PHE
1	B	257	LYS
1	B	262	ARG
1	B	285	LEU
1	B	304	LEU
1	B	317	VAL
1	B	324	ARG
1	B	429	PRO
1	B	431	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	159	GLN
1	A	305	GLN
1	A	336	GLN
1	A	418	ASN
1	B	45	ASN
1	B	71	ASN
1	B	159	GLN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	A	501	1,2	12,14,15	0.61	0	15,19,21	0.81	0
2	NAG	A	502	2	12,14,15	0.50	0	15,19,21	0.75	1 (6%)
3	NAG	A	601	1,3	12,14,15	0.61	0	15,19,21	0.83	0
3	NAG	A	602	3	12,14,15	0.43	0	15,19,21	0.97	1 (6%)
3	MAN	A	603	3	10,11,12	0.40	0	11,15,17	0.51	0
3	NAG	B	601	1,3	12,14,15	0.54	0	15,19,21	0.86	1 (6%)
3	NAG	B	602	3	12,14,15	0.53	0	15,19,21	1.00	1 (6%)
3	MAN	B	603	3	10,11,12	0.58	0	11,15,17	0.98	1 (9%)

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	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
3	MAN	A	603	3	-	0/2/19/22	0/1/1/1
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
3	MAN	B	603	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	MAN	C3-C4-C5	-2.36	105.99	110.20
3	B	601	NAG	C3-C2-N2	-2.23	108.37	111.76
3	A	602	NAG	C2-N2-C7	-2.22	119.36	123.09
3	B	602	NAG	C2-N2-C7	-2.16	119.46	123.09
2	A	502	NAG	C2-N2-C7	-2.04	119.66	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

4 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	#$|Z| > 2$
4	NAG	A	701	1	12,14,15	0.50	0	15,19,21	1.07	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	B	501	1	12,14,15	0.46	0	15,19,21	0.66	0
5	CIT	B	604	-	12,12,12	0.99	0	17,17,17	1.58	1 (5%)
5	CIT	B	605	-	12,12,12	2.36	5 (41%)	17,17,17	2.35	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	1/6/23/26	0/1/1/1
5	CIT	B	604	-	-	0/16/16/16	0/0/0/0
5	CIT	B	605	-	-	0/16/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	CIT	C2-C3	-5.09	1.47	1.53
5	B	605	CIT	C3-C6	3.90	1.57	1.53
5	B	605	CIT	C4-C5	3.40	1.62	1.50
5	B	605	CIT	O5-C6	-2.05	1.15	1.22
5	B	605	CIT	O4-C5	2.04	1.37	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	604	CIT	O6-C6-C3	5.06	120.25	112.89
5	B	605	CIT	O6-C6-C3	5.05	120.23	112.89
5	B	605	CIT	C4-C3-C2	-4.30	99.50	109.52
5	B	605	CIT	O4-C5-O3	-3.40	114.65	123.30
5	B	605	CIT	O5-C6-C3	-3.16	117.84	122.20
5	B	605	CIT	O7-C3-C4	2.72	114.70	109.22
5	B	605	CIT	O7-C3-C6	2.43	112.46	108.95
4	A	701	NAG	C3-C2-N2	-2.27	108.30	111.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	O7-C7-N2-C2

There are no ring outliers.

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(Å²)	Q<0.9
1	A	408/432 (94%)	-0.43	4 (0%)	79	79	14, 40, 63, 82	0
1	B	412/432 (95%)	-0.47	9 (2%)	59	60	16, 36, 58, 81	0
All	All	820/864 (94%)	-0.45	13 (1%)	68	69	14, 38, 61, 82	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	SER	3.2
1	B	43	ALA	2.9
1	B	44	THR	2.9
1	B	25	SER	2.6
1	A	44	THR	2.6
1	B	26	PRO	2.4
1	B	112	SER	2.3
1	B	400	VAL	2.2
1	A	12	PRO	2.2
1	B	397	PRO	2.1
1	A	25	SER	2.1
1	B	395	LEU	2.1
1	A	15	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	602	14/15	0.37	4.98	78,84,86,90	0
2	NAG	A	501	14/15	0.22	3.74	74,77,82,86	0
3	NAG	B	602	14/15	0.26	2.73	55,60,68,78	0
3	NAG	A	601	14/15	0.17	-0.18	52,59,64,70	0
3	NAG	B	601	14/15	0.14	-0.24	31,34,37,45	0
3	MAN	A	603	11/12	0.47	-	94,96,97,98	0
2	NAG	A	502	14/15	0.48	-	90,93,99,99	0
3	MAN	B	603	11/12	0.38	-	88,92,94,96	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CIT	B	605	13/13	0.34	18.59	118,118,120,120	0
4	NAG	A	701	14/15	0.41	17.29	77,81,82,82	0
4	NAG	B	501	14/15	0.23	8.79	58,61,65,65	0
5	CIT	B	604	13/13	0.38	4.00	132,133,133,134	0

6.5 Other polymers ⓘ

There are no such residues in this entry.