



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:23 AM UTC

PDB ID : 6NMB / pdb_00006nmb
Title : Tranexamic Acid is an Active Site Inhibitor of Urokinase Plasminogen Activator
Authors : Law, R.H.P.; Wu, G.
Deposited on : 2019-01-10
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

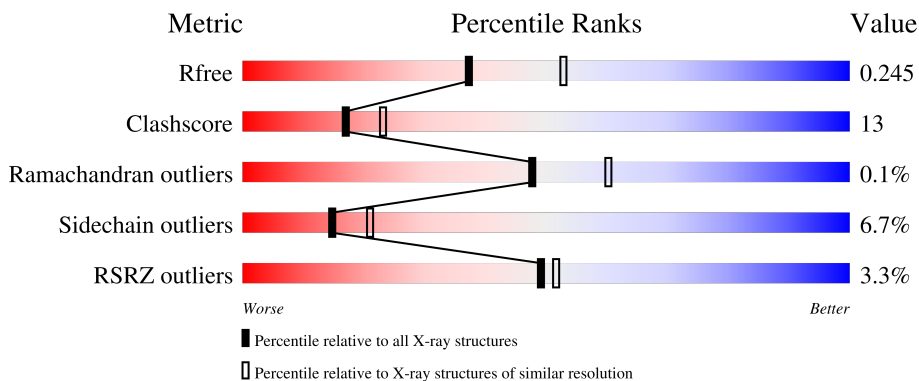
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	281	 2% 68% 19% • 11%
1	B	281	 2% 68% 21% • 10%
1	C	281	 4% 61% 25% • 10%
1	D	281	 3% 67% 21% • 11%

2 Entry composition [i](#)

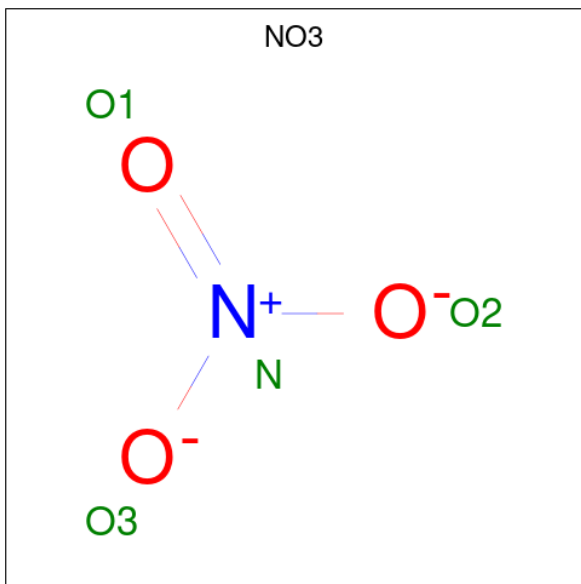
There are 4 unique types of molecules in this entry. The entry contains 8028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 1912	C 1212	N 319	O 364	S 17	0	0	0
1	B	254	Total 1936	C 1225	N 327	O 367	S 17	0	0	0
1	C	253	Total 1915	C 1212	N 322	O 364	S 17	0	0	0
1	D	251	Total 1903	C 1205	N 319	O 362	S 17	0	0	0

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



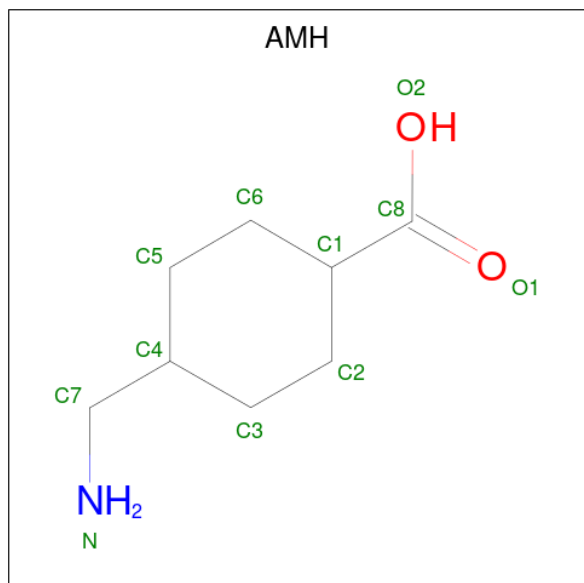
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	A	1	Total 4	N 1	O 3	0	0
2	B	1	Total 4	N 1	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is TRANS-4-AMINOMETHYLCYCLOHEXANE-1-CARBOXYLIC ACID (CCD ID: AMH) (formula: C₈H₁₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	8	1	2		
3	B	1	Total	C	N	O	0	0
			11	8	1	2		
3	C	1	Total	C	N	O	0	0
			11	8	1	2		
3	D	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	81	Total	O	0	1
			82	82		
4	C	68	Total	O	0	0
			68	68		

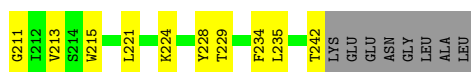
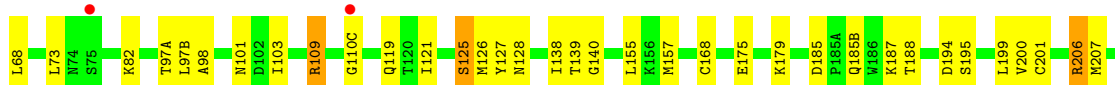
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	67	Total	O	0	0
			67	67		



• Molecule 1: Urokinase-type plasminogen activator



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.04Å 65.45Å 111.14Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	48.56 – 2.30 48.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.56-2.30) 77.4 (48.56-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.221 , 0.271 (Not available) , 0.245	Depositor DCC
R_{free} test set	1987 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.940	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6127e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: AMH, NO3

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	0.90	1/1961 (0.1%)	1.24	7/2667 (0.3%)
1	B	0.88	0/1985	1.22	5/2698 (0.2%)
1	C	0.89	1/1964 (0.1%)	1.23	6/2673 (0.2%)
1	D	0.88	2/1952 (0.1%)	1.25	7/2656 (0.3%)
All	All	0.89	4/7862 (0.1%)	1.24	25/10694 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	201	CYS	C-O	-5.73	1.16	1.23
1	C	58	CYS	C-O	-5.41	1.17	1.24
1	A	219	CYS	C-O	-5.38	1.17	1.24
1	D	109	ARG	C-O	5.25	1.30	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	125	SER	N-CA-C	-6.21	101.33	110.52
1	D	5	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	5	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	190	SER	N-CA-C	-5.99	101.61	110.48
1	D	97(B)	LEU	CA-C-N	5.99	129.61	121.05
1	D	97(B)	LEU	C-N-CA	5.99	129.61	121.05
1	D	140	GLY	N-CA-C	5.94	118.99	111.09
1	D	125	SER	N-CA-C	-5.93	102.55	110.55
1	A	189	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	176	VAL	N-CA-CB	5.67	117.47	111.00
1	C	61	LYS	CA-C-N	5.55	129.14	120.82
1	C	61	LYS	C-N-CA	5.55	129.14	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	VAL	CA-C-N	5.49	128.19	120.28
1	A	85	VAL	C-N-CA	5.49	128.19	120.28
1	B	125	SER	N-CA-C	-5.49	101.59	110.32
1	B	61	LYS	CA-C-N	5.47	131.98	121.54
1	B	61	LYS	C-N-CA	5.47	131.98	121.54
1	B	148	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	194	ASP	CA-C-N	5.37	129.31	121.31
1	D	194	ASP	C-N-CA	5.37	129.31	121.31
1	A	48	SER	CA-C-O	-5.36	115.68	120.56
1	A	125	SER	N-CA-C	-5.34	102.62	110.52
1	C	190	SER	N-CA-C	-5.33	102.59	110.48
1	C	48	SER	CA-C-O	-5.23	116.16	120.71

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	1912	0	1791	32	0
1	B	1936	0	1811	50	0
1	C	1915	0	1776	65	0
1	D	1903	0	1771	43	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	11	0	14	0	0
3	B	11	0	14	0	0
3	C	11	0	14	0	0
3	D	11	0	14	0	0
4	A	85	0	0	3	0
4	B	82	0	0	3	0
4	C	68	0	0	3	0
4	D	67	0	0	1	0
All	All	8028	0	7205	190	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 13.

All (190) 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:B:230:ARG:HD3	1:B:233:HIS:CD2	1.77	1.19
1:C:10:LYS:HD3	1:C:10:LYS:C	1.77	1.06
1:D:56:THR:HG22	1:D:103:ILE:O	1.64	0.96
1:B:200:VAL:HG12	1:B:207:MET:HE3	1.49	0.93
1:B:181:LEU:HG	1:B:230:ARG:NH1	1.88	0.89
1:C:7:CYS:HA	1:C:120:THR:HG22	1.58	0.86
1:A:97(A):THR:HG23	1:A:175:GLU:OE1	1.78	0.84
1:B:200:VAL:CG1	1:B:207:MET:HE3	2.07	0.84
1:A:206:ARG:HD3	4:A:459:HOH:O	1.78	0.82
1:D:200:VAL:HG12	1:D:207:MET:HE3	1.61	0.82
1:B:42:CYS:HB2	1:B:195:SER:O	1.78	0.82
1:B:230:ARG:CD	1:B:233:HIS:CD2	2.64	0.79
1:C:56:THR:HG21	1:C:91:HIS:H	1.48	0.78
1:C:35:ARG:NE	1:C:60(B):TYR:CD1	2.51	0.78
1:B:97(A):THR:HG23	1:B:175:GLU:OE1	1.83	0.77
1:D:67:TYR:OH	1:D:82:LYS:HD2	1.84	0.77
1:B:181:LEU:HG	1:B:230:ARG:HH11	1.49	0.77
1:C:68:LEU:HD13	1:C:83:PHE:CD1	2.19	0.77
1:B:120:THR:HG21	4:B:471:HOH:O	1.85	0.75
1:C:51:TRP:CZ2	1:C:107:LYS:HD2	2.22	0.75
1:B:7:CYS:HA	1:B:120:THR:HG22	1.70	0.74
1:C:68:LEU:HD13	1:C:83:PHE:CE1	2.23	0.73
1:D:98:ALA:HB2	1:D:175:GLU:HG3	1.71	0.71
1:A:42:CYS:HB2	1:A:195:SER:O	1.91	0.71
1:D:206:ARG:HB2	1:D:206:ARG:HH11	1.56	0.70
1:C:7:CYS:CA	1:C:120:THR:HG22	2.23	0.69
1:B:68:LEU:HD13	1:B:83:PHE:CE1	2.29	0.68
1:D:56:THR:CG2	1:D:103:ILE:O	2.40	0.68
1:D:200:VAL:CG1	1:D:207:MET:HE3	2.23	0.68
1:D:185(B):GLN:O	1:D:187:LYS:HE2	1.93	0.68
1:C:7:CYS:CB	1:C:120:THR:CG2	2.73	0.67
1:A:126:MET:HG2	1:A:127:TYR:CD2	2.29	0.67
1:C:22:THR:O	1:C:154:GLN:NE2	2.28	0.66
1:A:140:GLY:HA3	1:A:194:ASP:OD1	1.96	0.66
1:D:42:CYS:HB2	1:D:195:SER:O	1.96	0.65
1:C:18:GLY:HA3	1:C:188:THR:CG2	2.26	0.65
1:B:68:LEU:HD13	1:B:83:PHE:CD1	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97(A):THR:CG2	1:A:175:GLU:OE1	2.45	0.65
1:C:67:TYR:OH	1:C:82:LYS:HD2	1.97	0.64
1:C:56:THR:HG23	1:C:103:ILE:O	1.99	0.63
1:D:101:ASN:HD22	1:D:234:PHE:HE2	1.45	0.63
1:C:5:PHE:HE1	1:C:119:GLN:HA	1.62	0.63
1:A:184:ALA:HB2	1:A:225:PRO:HB3	1.81	0.62
1:C:160:VAL:HG13	1:C:183:ALA:HB1	1.82	0.61
1:C:17:ILE:O	1:C:188:THR:HG22	2.00	0.61
1:B:181:LEU:CD2	1:B:230:ARG:HH12	2.14	0.60
1:C:56:THR:CG2	1:C:103:ILE:O	2.50	0.60
1:C:126:MET:HA	1:C:235:LEU:HD22	1.84	0.60
1:A:74:ASN:ND2	1:A:153:GLU:OE2	2.35	0.59
1:C:98:ALA:HB2	1:C:175:GLU:HG3	1.82	0.59
1:C:172:TYR:CE1	1:C:224:LYS:HD2	2.36	0.59
1:B:62:LYS:HB2	4:B:444:HOH:O	2.03	0.59
1:B:51:TRP:CZ2	1:B:107:LYS:HD2	2.36	0.59
1:B:221:LEU:HB2	4:B:423:HOH:O	2.03	0.59
1:C:206:ARG:HG3	1:C:206:ARG:HH21	1.69	0.58
1:C:5:PHE:CE1	1:C:119:GLN:HA	2.39	0.58
1:D:56:THR:HG22	1:D:103:ILE:C	2.29	0.57
1:C:7:CYS:HB3	1:C:120:THR:CG2	2.35	0.57
1:B:185(B):GLN:O	1:B:187:LYS:HD3	2.04	0.57
1:D:126:MET:HG2	1:D:127:TYR:CD2	2.40	0.57
1:C:7:CYS:CB	1:C:120:THR:HG22	2.35	0.56
1:A:169:GLN:HG3	1:A:176:VAL:HG22	1.87	0.56
1:D:200:VAL:HG12	1:D:207:MET:CE	2.34	0.56
1:A:81:MET:HG3	4:A:462:HOH:O	2.05	0.56
1:B:181:LEU:CG	1:B:230:ARG:NH1	2.64	0.56
1:C:35:ARG:HB2	1:C:41:VAL:HG21	1.86	0.56
1:D:64:TYR:O	1:D:65:ILE:HD13	2.06	0.56
1:C:132:PHE:CE2	1:C:164:SER:HA	2.41	0.55
1:C:56:THR:HG22	1:C:104:ALA:HB2	1.87	0.55
1:A:24:ILE:HD11	1:A:30:PHE:HB3	1.87	0.55
1:B:19:GLY:HA3	1:B:158:THR:HB	1.88	0.55
1:C:181:LEU:HD21	1:C:230:ARG:NE	2.21	0.55
1:A:125:SER:OG	1:A:128:ASN:ND2	2.37	0.55
1:B:46:LEU:O	1:B:121:ILE:HG22	2.07	0.54
1:C:18:GLY:HA3	1:C:188:THR:HG23	1.90	0.54
1:B:151:TYR:HE1	1:B:193:GLY:HA3	1.72	0.54
1:B:164:SER:OG	1:B:166:ARG:HG3	2.07	0.54
1:C:158:THR:OG1	1:C:188:THR:HG21	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD12	1:A:43:GLY:O	2.07	0.54
1:B:230:ARG:HD3	1:B:233:HIS:CG	2.38	0.54
1:D:28:PRO:HB2	1:D:119:GLN:HB3	1.90	0.54
1:C:18:GLY:HA3	1:C:188:THR:HG22	1.89	0.54
1:D:185:ASP:HB2	1:D:188:THR:HG22	1.89	0.53
1:B:126:MET:HG2	1:B:127:TYR:CD2	2.44	0.53
1:C:126:MET:HG2	1:C:127:TYR:CD2	2.43	0.53
1:D:51:TRP:CE2	1:D:242:THR:HG22	2.44	0.53
1:C:126:MET:HG2	1:C:127:TYR:CE2	2.43	0.53
1:D:206:ARG:HH11	1:D:206:ARG:CB	2.21	0.52
1:A:137:GLU:HB2	1:A:200:VAL:HG23	1.92	0.52
1:D:139:THR:HG22	1:D:155:LEU:HD11	1.92	0.52
1:C:35:ARG:NE	1:C:60(B):TYR:CE1	2.77	0.52
1:A:26:ASN:HB3	1:A:157:MET:HE1	1.92	0.52
1:C:48:SER:HB3	4:C:429:HOH:O	2.10	0.51
1:C:121:ILE:HD11	1:C:200:VAL:HG22	1.92	0.51
1:B:110(D):ARG:HD2	1:B:113:GLN:NE2	2.25	0.51
1:B:166:ARG:HG3	1:B:167:GLU:H	1.74	0.51
1:A:151:TYR:HE2	1:A:193:GLY:HA3	1.74	0.51
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.75	0.51
1:B:170(B):HIS:H	1:B:170(B):HIS:CD2	2.28	0.51
1:C:166:ARG:HG2	1:C:167:GLU:N	2.26	0.51
1:C:172:TYR:HE1	1:C:224:LYS:HD2	1.76	0.50
1:C:86:GLU:OE1	1:C:109:ARG:HD3	2.12	0.50
1:D:121:ILE:HD11	1:D:200:VAL:HG22	1.92	0.50
1:C:51:TRP:CE2	1:C:107:LYS:HD2	2.46	0.50
1:D:16:ILE:HD12	1:D:138:ILE:HD12	1.93	0.50
1:B:71:SER:H	1:B:77:THR:HG21	1.77	0.50
1:D:97(A):THR:OG1	1:D:175:GLU:OE2	2.29	0.50
1:A:71:SER:H	1:A:77:THR:HG21	1.76	0.49
1:D:126:MET:HG2	1:D:127:TYR:CE2	2.47	0.49
1:C:88:LEU:HG	1:C:90:LEU:HD21	1.94	0.49
1:D:67:TYR:OH	1:D:82:LYS:CD	2.58	0.49
1:D:10:LYS:HD2	1:D:207:MET:SD	2.52	0.49
1:D:121:ILE:CD1	1:D:200:VAL:HG22	2.43	0.49
1:D:126:MET:HA	1:D:235:LEU:HD22	1.93	0.49
1:D:64:TYR:C	1:D:65:ILE:HD13	2.37	0.49
1:B:4:LYS:N	1:B:114:PRO:HG3	2.28	0.49
1:A:51:TRP:CE2	1:A:242:THR:HG22	2.48	0.48
1:A:126:MET:HG2	1:A:127:TYR:CE2	2.48	0.48
1:B:24:ILE:CG2	1:B:117:THR:HB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:HG3	1:C:85:VAL:O	2.14	0.48
1:D:109:ARG:HD3	1:D:110(C):GLY:HA2	1.96	0.47
1:D:67:TYR:CZ	1:D:82:LYS:HD2	2.49	0.47
1:D:125:SER:OG	1:D:128:ASN:ND2	2.46	0.47
1:B:230:ARG:NH1	1:B:230:ARG:HG3	2.29	0.47
1:B:7:CYS:HA	1:B:120:THR:CG2	2.43	0.46
1:D:46:LEU:HD13	1:D:68:LEU:HD11	1.97	0.46
1:A:19:GLY:HA3	1:A:158:THR:HB	1.98	0.46
1:C:213:VAL:HG22	1:C:228:TYR:HE2	1.80	0.46
1:B:110(D):ARG:HD2	1:B:113:GLN:HE22	1.81	0.45
1:C:156:LYS:HB3	1:C:156:LYS:HE2	1.81	0.45
1:A:6:GLN:O	1:A:6:GLN:HG3	2.17	0.45
1:B:45:SER:OG	1:B:198:PRO:HB3	2.16	0.45
1:C:213:VAL:HG22	1:C:228:TYR:CE2	2.51	0.45
1:A:53:ILE:HD11	1:A:103:ILE:HD11	1.99	0.45
1:A:213:VAL:HG22	1:A:228:TYR:HE2	1.82	0.45
1:B:230:ARG:NE	1:B:233:HIS:NE2	2.65	0.45
1:A:62:LYS:HE3	1:A:62:LYS:HB3	1.65	0.45
1:B:46:LEU:HD13	1:B:68:LEU:HD21	1.98	0.45
1:B:53:ILE:HD11	1:B:103:ILE:HD11	1.98	0.44
1:C:221:LEU:HB2	1:C:224:LYS:HB2	1.98	0.44
1:A:67:TYR:OH	1:A:82:LYS:HD2	2.16	0.44
1:B:17:ILE:HD11	1:B:191:CYS:SG	2.58	0.44
1:A:27:GLN:HE21	1:A:157:MET:HE2	1.82	0.44
1:A:139:THR:HG22	1:A:155:LEU:HD11	1.99	0.43
1:C:16:ILE:N	1:C:142:GLY:O	2.51	0.43
1:B:49:PRO:O	1:B:111:CYS:HB3	2.18	0.43
1:B:140:GLY:HA3	1:B:194:ASP:OD1	2.18	0.43
1:D:221:LEU:HB2	1:D:224:LYS:HB2	2.01	0.43
1:C:126:MET:HE3	4:C:466:HOH:O	2.18	0.43
1:D:98:ALA:HA	1:D:215:TRP:CE2	2.53	0.43
1:C:109:ARG:HG3	4:C:449:HOH:O	2.19	0.43
1:C:121:ILE:CD1	1:C:200:VAL:HG22	2.47	0.43
1:C:19:GLY:HA3	1:C:158:THR:HB	2.01	0.43
1:D:213:VAL:HG22	1:D:228:TYR:HE2	1.84	0.43
1:B:62:LYS:HG2	1:B:85:VAL:O	2.19	0.42
1:B:218:GLY:HA3	1:B:221:LEU:HD22	2.01	0.42
1:C:139:THR:HG22	1:C:155:LEU:HD11	2.02	0.42
1:B:200:VAL:HG12	1:B:207:MET:CE	2.36	0.42
1:C:51:TRP:CZ2	1:C:107:LYS:CD	2.99	0.42
1:A:186:TRP:CG	1:A:222:LYS:HA	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD12	1:B:207:MET:O	2.20	0.42
1:A:5:PHE:CD1	1:A:114:PRO:HB3	2.54	0.42
1:A:40:TYR:HE2	4:A:407:HOH:O	2.00	0.42
1:A:137:GLU:HB2	1:A:200:VAL:CG2	2.49	0.42
1:C:51:TRP:CZ3	1:C:107:LYS:HB2	2.55	0.42
1:C:160:VAL:HG22	1:C:184:ALA:CA	2.49	0.42
1:D:206:ARG:HH11	1:D:206:ARG:CG	2.32	0.41
1:C:67:TYR:CZ	1:C:82:LYS:HD2	2.54	0.41
1:B:162:LEU:HD21	1:B:199:LEU:HD11	2.02	0.41
1:A:27:GLN:HE21	1:A:157:MET:CE	2.33	0.41
1:C:232:SER:HA	1:C:235:LEU:HD13	2.02	0.41
1:D:139:THR:O	4:D:401:HOH:O	2.22	0.41
1:C:160:VAL:HG22	1:C:184:ALA:HA	2.03	0.41
1:C:206:ARG:HG3	1:C:206:ARG:NH2	2.35	0.41
1:B:7:CYS:CA	1:B:120:THR:HG22	2.43	0.41
1:B:97(A):THR:CG2	1:B:175:GLU:OE1	2.63	0.41
1:C:7:CYS:HB2	1:C:120:THR:CG2	2.48	0.41
1:C:199:LEU:HB3	1:C:211:GLY:CA	2.51	0.41
1:C:22:THR:HG21	1:C:157:MET:SD	2.60	0.41
1:B:181:LEU:CD2	1:B:230:ARG:NH1	2.78	0.40
1:C:132:PHE:CD2	1:C:164:SER:HA	2.56	0.40
1:D:211:GLY:HA2	1:D:229:THR:O	2.21	0.40
1:B:7:CYS:CB	1:B:120:THR:HG23	2.51	0.40
1:D:33:ILE:HD12	1:D:43:GLY:O	2.22	0.40
1:D:179:LYS:HB3	1:D:234:PHE:CE1	2.56	0.40
1:C:35:ARG:HB2	1:C:41:VAL:CG2	2.48	0.40
1:D:29:TRP:HA	1:D:119:GLN:O	2.22	0.40
1:D:40:TYR:CE2	1:D:42:CYS:HA	2.56	0.40
1:C:77:THR:O	1:C:80:GLU:HB3	2.21	0.40
1:D:199:LEU:HD22	1:D:228:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/281 (88%)	234 (95%)	13 (5%)	0	100	100
1	B	250/281 (89%)	238 (95%)	12 (5%)	0	100	100
1	C	249/281 (89%)	230 (92%)	18 (7%)	1 (0%)	30	38
1	D	247/281 (88%)	230 (93%)	17 (7%)	0	100	100
All	All	993/1124 (88%)	932 (94%)	60 (6%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110(C)	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/247 (83%)	193 (94%)	12 (6%)	18	26
1	B	206/247 (83%)	194 (94%)	12 (6%)	18	26
1	C	202/247 (82%)	181 (90%)	21 (10%)	7	8
1	D	202/247 (82%)	192 (95%)	10 (5%)	22	33
All	All	815/988 (82%)	760 (93%)	55 (7%)	15	21

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	38	VAL
1	A	62	LYS
1	A	62(A)	GLU
1	A	71	SER
1	A	77	THR
1	A	84	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	166	ARG
1	A	168	CYS
1	A	176	VAL
1	A	178	THR
1	A	221	LEU
1	B	16	ILE
1	B	24	ILE
1	B	56	THR
1	B	77	THR
1	B	109	ARG
1	B	120	THR
1	B	154	GLN
1	B	160	VAL
1	B	168	CYS
1	B	199	LEU
1	B	202	SER
1	B	221	LEU
1	C	6	GLN
1	C	10	LYS
1	C	16	ILE
1	C	22	THR
1	C	23	THR
1	C	47	ILE
1	C	48	SER
1	C	62	LYS
1	C	62(A)	GLU
1	C	65	ILE
1	C	75	SER
1	C	113	GLN
1	C	120	THR
1	C	125	SER
1	C	160	VAL
1	C	166	ARG
1	C	168	CYS
1	C	188	THR
1	C	206	ARG
1	C	227	VAL
1	C	240	SER
1	D	25	GLU
1	D	45	SER
1	D	48	SER
1	D	56	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	63	ASP
1	D	65	ILE
1	D	73	LEU
1	D	157	MET
1	D	168	CYS
1	D	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	128	ASN
1	A	241	HIS
1	B	74	ASN
1	B	76	ASN
1	B	154	GLN
1	B	170	GLN
1	B	170(B)	HIS
1	C	74	ASN
1	C	100	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	NO3	A	301	-	1,3,3	0.50	0	0,3,3	-	-
3	AMH	A	302	-	10,11,11	1.21	0	13,14,14	1.33	2 (15%)
2	NO3	D	301	-	1,3,3	0.59	0	0,3,3	-	-
3	AMH	B	302	-	10,11,11	1.18	1 (10%)	13,14,14	1.90	5 (38%)
2	NO3	C	301	-	1,3,3	0.57	0	0,3,3	-	-
2	NO3	B	301	-	1,3,3	0.48	0	0,3,3	-	-
3	AMH	C	302	-	10,11,11	1.27	1 (10%)	13,14,14	1.64	2 (15%)
3	AMH	D	302	-	10,11,11	1.45	2 (20%)	13,14,14	1.34	1 (7%)

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	AMH	A	302	-	-	3/6/16/16	0/1/1/1
3	AMH	C	302	-	-	0/6/16/16	0/1/1/1
3	AMH	D	302	-	-	0/6/16/16	1/1/1/1
3	AMH	B	302	-	-	0/6/16/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	AMH	C1-C8	2.40	1.55	1.51
3	B	302	AMH	C6-C1	2.24	1.58	1.53
3	D	302	AMH	C6-C1	2.14	1.58	1.53
3	C	302	AMH	C1-C8	2.04	1.55	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	AMH	C6-C1-C2	4.37	119.20	110.00
3	C	302	AMH	C5-C4-C3	2.97	116.54	109.29
3	B	302	AMH	O1-C8-C1	-2.76	115.54	122.86
3	A	302	AMH	C5-C4-C3	2.65	115.77	109.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	AMH	O1-C8-C1	-2.62	115.91	122.86
3	D	302	AMH	O1-C8-C1	-2.43	116.42	122.86
3	B	302	AMH	C5-C6-C1	2.19	115.04	111.18
3	B	302	AMH	C6-C1-C8	2.14	115.68	111.28
3	B	302	AMH	C2-C3-C4	-2.12	108.35	112.36
3	C	302	AMH	C5-C6-C1	2.11	114.90	111.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	AMH	C5-C4-C7-N
3	A	302	AMH	C3-C4-C7-N
3	A	302	AMH	C6-C1-C8-O1

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302	AMH	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	251/281 (89%)	0.41	7 (2%) 55 57	16, 26, 47, 72	0
1	B	254/281 (90%)	0.40	7 (2%) 55 57	12, 26, 51, 75	0
1	C	253/281 (90%)	0.53	11 (4%) 40 41	17, 28, 55, 84	0
1	D	251/281 (89%)	0.42	8 (3%) 50 52	14, 27, 51, 89	0
All	All	1009/1124 (89%)	0.44	33 (3%) 49 51	12, 27, 52, 89	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37(A)	ARG	4.8
1	B	11	THR	4.7
1	D	37(B)	GLY	3.5
1	A	37	HIS	3.5
1	A	37(A)	ARG	3.3
1	B	9	GLN	3.2
1	A	37(C)	GLY	3.1
1	D	110(C)	GLY	3.1
1	D	60(B)	TYR	3.1
1	C	37(B)	GLY	3.1
1	B	4	LYS	2.9
1	A	37(B)	GLY	2.9
1	D	37(C)	GLY	2.8
1	C	37(C)	GLY	2.8
1	C	10	LYS	2.8
1	C	5	PHE	2.7
1	B	243	LYS	2.7
1	C	37	HIS	2.6
1	D	37(A)	ARG	2.6
1	B	132	PHE	2.4
1	D	10	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.3
1	A	37(D)	SER	2.3
1	C	60(B)	TYR	2.2
1	A	60(B)	TYR	2.2
1	D	75	SER	2.2
1	D	37	HIS	2.2
1	C	188	THR	2.2
1	C	119	GLN	2.1
1	B	37(A)	ARG	2.1
1	C	4	LYS	2.1
1	B	10	LYS	2.0
1	C	37(D)	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NO3	C	301	4/4	0.77	0.13	41,43,43,43	0
2	NO3	B	301	4/4	0.79	0.15	46,46,47,47	0
3	AMH	C	302	11/11	0.80	0.15	30,34,37,40	0
2	NO3	A	301	4/4	0.85	0.12	44,44,45,46	0
3	AMH	D	302	11/11	0.85	0.13	25,28,33,39	0
3	AMH	A	302	11/11	0.87	0.12	24,27,36,43	0
3	AMH	B	302	11/11	0.88	0.13	29,31,39,43	0
2	NO3	D	301	4/4	0.95	0.06	44,44,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.