



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2A0Q / pdb_00002a0q
Title : Structure of thrombin in 400 mM potassium chloride
Authors : Papaconstantinou, M.; Carrell, C.J.; Pineda, A.O.; Bobofchak, K.M.; Mathews, F.S.; Flordellis, C.S.; Maragoudakis, M.E.; Tsopanoglou, N.E.; di Cera, E.
Deposited on : 2005-06-16
Resolution : 1.90 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

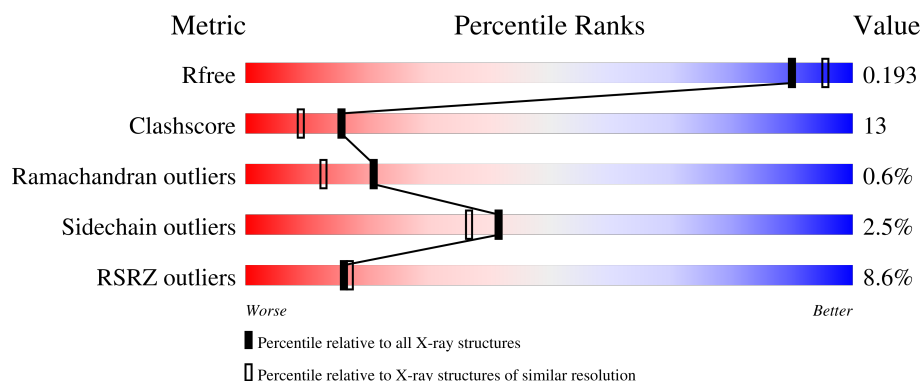
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	30	10% 70% 30%
1	C	30	17% 67% 27% 7%
2	B	257	3% 75% 18% 6%
2	D	257	12% 61% 31% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4749 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 Thrombin, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	30	Total	C	N	O	S	0	0	0
			246	152	42	51	1			
1	C	28	Total	C	N	O	S	0	0	0
			230	144	37	48	1			

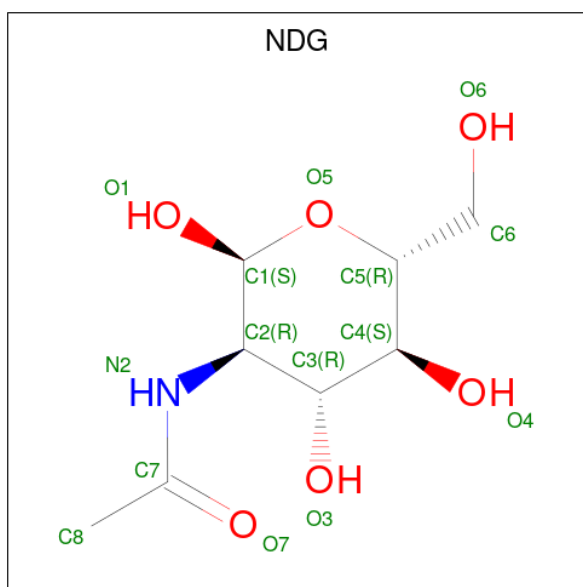
- Molecule 2 is a protein called Thrombin, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1959	1252	344	349	14			
2	D	245	Total	C	N	O	S	0	0	0
			1985	1271	347	353	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77A	ALA	ARG	engineered mutation	UNP P00734
D	77A	ALA	ARG	engineered mutation	UNP P00734

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	168	Total	O	0	0
			168	168		
6	C	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	115	Total 115	O 115	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 69.74Å 158.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 1.90 29.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.40-1.90) 91.6 (29.40-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.240 0.193 , 0.193	Depositor DCC
R_{free} test set	2464 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4749	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NDG, K

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	0.68	0/248	1.10	3/328 (0.9%)
1	C	0.65	0/232	1.17	2/309 (0.6%)
2	B	0.69	1/2010 (0.0%)	1.07	5/2715 (0.2%)
2	D	0.58	0/2036	1.11	9/2750 (0.3%)
All	All	0.64	1/4526 (0.0%)	1.10	19/6102 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	MET	SD-CE	-5.48	1.65	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14(K)	ILE	N-CA-C	-9.08	104.63	113.53
2	B	35	ARG	N-CA-C	-7.21	98.81	110.20
2	B	60(B)	PRO	N-CA-C	6.75	118.94	110.70
2	D	60(I)	THR	N-CA-C	-6.74	100.24	110.14
1	C	14(A)	LYS	N-CA-C	6.71	119.42	111.71
2	D	35	ARG	N-CA-C	-6.41	100.07	110.20
2	D	76	TYR	N-CA-C	-6.30	97.43	108.20
1	A	14(A)	LYS	N-CA-C	6.22	120.12	112.54
1	A	14(L)	ASP	N-CA-C	6.18	120.99	112.90
2	B	64	LEU	N-CA-C	5.90	118.15	109.24
2	D	123	LEU	N-CA-C	-5.85	102.22	110.29
2	D	143	ASN	N-CA-C	5.75	121.00	113.30
2	D	43	GLY	N-CA-C	-5.69	103.90	112.60
2	D	192	GLU	N-CA-C	-5.60	102.73	110.35
1	A	1(A)	ASP	N-CA-C	-5.58	105.82	113.30
2	B	125	ASP	N-CA-C	-5.57	101.67	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	HIS	N-CA-C	-5.46	105.92	113.18
2	D	144	LEU	N-CA-C	5.36	118.08	110.10
2	D	60(H)	PHE	N-CA-C	5.25	117.07	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	246	0	245	5	0
1	C	230	0	229	7	0
2	B	1959	0	1932	31	0
2	D	1985	0	1965	78	0
3	B	15	0	12	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	0	0
6	B	168	0	0	3	0
6	C	8	0	0	0	0
6	D	115	0	0	4	0
All	All	4749	0	4383	117	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 (117) 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)
2:D:173:ARG:HH11	2:D:173:ARG:HB3	1.28	0.97
2:D:95:ASN:HD21	2:D:97(A):GLU:HB3	1.28	0.93
2:D:50:ARG:NH1	2:D:107:LYS:HE3	1.90	0.86
2:B:202:LYS:HE2	2:B:205:ASN:ND2	1.98	0.79
2:B:26:MET:HE1	6:B:543:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:GLN:O	2:D:245:PHE:HB2	1.86	0.75
2:D:67:ARG:HD2	2:D:80:GLU:OE1	1.85	0.75
1:C:10:LYS:HZ2	1:C:12:LEU:HD22	1.50	0.75
2:D:34:PHE:HB2	2:D:65:LEU:CD2	2.17	0.74
2:D:95:ASN:HD21	2:D:97(A):GLU:CB	2.01	0.72
2:D:173:ARG:HB3	2:D:173:ARG:NH1	2.04	0.72
2:D:95:ASN:ND2	2:D:97(A):GLU:HB3	2.06	0.69
1:C:14:ASP:HB2	2:D:26:MET:HE3	1.74	0.69
2:D:169:LYS:HE3	2:D:176:ILE:HG12	1.76	0.68
1:C:10:LYS:O	1:C:12:LEU:HD13	1.94	0.68
2:B:138:VAL:HG11	2:B:190:ALA:HB2	1.77	0.66
2:D:236:LYS:HA	2:D:236:LYS:HZ3	1.61	0.65
2:D:186(C):GLY:O	2:D:186(D):LYS:HD2	1.96	0.64
2:D:186(A):ASP:CG	2:D:186(B):GLU:H	2.05	0.63
1:A:10:LYS:O	1:A:12:LEU:HD13	1.98	0.63
1:C:10:LYS:HZ2	1:C:12:LEU:CD2	2.12	0.62
2:D:34:PHE:HB2	2:D:65:LEU:HD23	1.81	0.62
2:B:75:ARG:NH1	2:B:77:GLU:HG2	2.15	0.62
2:B:88:ILE:CD1	2:B:106:MET:HG2	2.31	0.61
2:D:87:LYS:HG2	2:D:89:TYR:CZ	2.35	0.61
2:B:36(A):SER:HA	2:B:37:PRO:C	2.24	0.61
1:A:13:GLU:CD	1:A:14(D):ARG:HH21	2.09	0.59
2:D:151:GLN:N	2:D:152:PRO:HD3	2.18	0.59
2:B:88:ILE:HD13	2:B:106:MET:HG2	1.84	0.59
2:D:50:ARG:HH11	2:D:107:LYS:HE3	1.67	0.58
2:D:100:ASP:OD2	2:D:101:ARG:NH1	2.36	0.58
1:A:14:ASP:HB2	2:B:26:MET:HE2	1.84	0.58
2:D:50:ARG:HD3	2:D:108:LEU:O	2.04	0.57
1:C:14(H):GLU:O	1:C:14(L):ASP:HB2	2.05	0.56
2:B:244:GLN:O	2:B:245:PHE:HB2	2.06	0.56
2:D:87:LYS:HG3	2:D:88:ILE:N	2.20	0.56
2:D:91:HIS:CE1	2:D:101:ARG:HD3	2.41	0.56
2:D:60(B):PRO:HG2	2:D:96:TRP:CZ2	2.41	0.55
2:B:235:LYS:HE2	2:B:239:GLN:OE1	2.06	0.55
2:B:236:LYS:HB2	6:B:516:HOH:O	2.06	0.54
2:D:169:LYS:HG2	2:D:176:ILE:HD11	1.89	0.54
2:D:224:LYS:N	2:D:224:LYS:HE3	2.22	0.54
2:D:184(A):TYR:CD2	2:D:186(D):LYS:HB3	2.43	0.54
2:B:32:MET:SD	2:B:70:LYS:HD3	2.48	0.53
2:B:91:HIS:CE1	2:B:101:ARG:HD3	2.43	0.53
2:B:67:ARG:HD2	2:B:70:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:GLU:HG2	2:D:87:LYS:HA	1.88	0.53
1:C:14(D):ARG:O	1:C:14(H):GLU:HG3	2.08	0.53
2:D:236:LYS:NZ	2:D:239:GLN:HE21	2.07	0.53
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.16	0.53
2:D:204(B):ASN:HD22	2:D:204(B):ASN:C	2.17	0.53
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.90	0.52
2:D:204(B):ASN:ND2	2:D:206:ARG:H	2.07	0.52
2:D:77(A):ALA:O	2:D:78:ASN:HB2	2.09	0.52
2:D:186(A):ASP:O	2:D:186(B):GLU:C	2.53	0.52
2:D:32:MET:SD	2:D:70:LYS:HD3	2.50	0.51
2:B:61:GLU:CG	2:B:87:LYS:HA	2.40	0.51
2:D:230:HIS:CG	2:D:233:ARG:HG3	2.46	0.51
2:D:124:PRO:HB3	2:D:210:MET:SD	2.53	0.49
2:D:186(A):ASP:O	2:D:186(C):GLY:N	2.46	0.49
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.11	0.49
2:D:130:LEU:CD2	2:D:230:HIS:NE2	2.76	0.49
2:D:163:VAL:HB	2:D:168:CYS:SG	2.53	0.48
2:D:136:GLY:HA3	2:D:199:PHE:CZ	2.48	0.48
2:D:236:LYS:HZ3	2:D:239:GLN:HE21	1.62	0.48
2:B:187:ARG:HG3	2:D:145:LYS:HB3	1.95	0.48
2:D:60(A):TYR:CE2	2:D:60(C):PRO:HB2	2.48	0.48
2:B:16:ILE:N	2:B:194:ASP:OD2	2.45	0.48
2:D:169:LYS:HE3	2:D:176:ILE:CG1	2.42	0.47
1:C:10:LYS:NZ	1:C:12:LEU:CD2	2.77	0.47
2:D:224:LYS:HE3	2:D:224:LYS:CA	2.44	0.47
2:D:137:ARG:HG3	2:D:157:VAL:HG23	1.97	0.47
2:D:224:LYS:N	6:D:473:HOH:O	2.48	0.47
2:D:124:PRO:HD3	2:D:209:GLN:O	2.16	0.46
2:D:244:GLN:O	2:D:245:PHE:CB	2.60	0.46
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.51	0.45
2:B:221(A):ARG:NH2	2:D:220:CYS:HB3	2.31	0.45
2:D:100:ASP:OD1	2:D:177:THR:OG1	2.31	0.45
2:D:79:ILE:HD12	2:D:117:TYR:CD2	2.52	0.45
2:D:147:THR:HG22	2:D:147:THR:O	2.15	0.45
2:B:23:GLU:OE2	2:B:26:MET:CE	2.64	0.45
2:D:61:GLU:CD	2:D:61:GLU:H	2.24	0.44
2:D:224:LYS:N	2:D:224:LYS:CE	2.81	0.44
2:B:17:VAL:HG12	2:B:18:GLU:HG2	2.00	0.43
2:D:61:GLU:CG	2:D:87:LYS:HA	2.48	0.43
2:D:186(A):ASP:CG	2:D:186(B):GLU:N	2.75	0.43
1:A:14(D):ARG:HH11	1:A:14(D):ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ARG:HD2	2:D:107:LYS:NZ	2.33	0.43
2:D:77(A):ALA:O	2:D:78:ASN:CB	2.67	0.43
2:D:163:VAL:HB	2:D:182:CYS:SG	2.59	0.43
2:B:203:SER:HB3	2:B:204(B):ASN:ND2	2.34	0.43
2:D:60(A):TYR:C	2:D:60(C):PRO:HD2	2.44	0.42
2:D:80:GLU:C	2:D:81:LYS:HD2	2.44	0.42
2:B:87:LYS:HE2	6:B:489:HOH:O	2.19	0.42
2:B:129:ALA:HA	2:B:210:MET:HE1	2.02	0.42
2:D:176:ILE:HG21	2:D:227:PHE:CE2	2.54	0.42
2:D:224:LYS:N	2:D:224:LYS:CD	2.81	0.42
2:D:184(A):TYR:CZ	2:D:186(D):LYS:HG2	2.55	0.42
2:D:237:TRP:HA	2:D:240:LYS:HE2	1.99	0.42
2:D:186(B):GLU:O	2:D:186(C):GLY:C	2.63	0.42
2:B:29:TRP:CG	2:B:121:VAL:HB	2.54	0.42
2:D:211:GLY:HA2	2:D:229:THR:O	2.20	0.42
2:B:18:GLU:HB2	2:B:188:GLY:HA2	2.01	0.41
1:A:14(D):ARG:HH12	1:A:14(G):LEU:HD12	1.85	0.41
2:D:169:LYS:HG2	2:D:176:ILE:CD1	2.49	0.41
2:D:236:LYS:NZ	2:D:239:GLN:NE2	2.69	0.41
2:D:186(C):GLY:HA2	6:D:490:HOH:O	2.21	0.41
2:D:176:ILE:O	2:D:176:ILE:HG13	2.20	0.41
2:D:18:GLU:OE2	2:D:187:ARG:HD3	2.20	0.41
2:D:29:TRP:CG	2:D:121:VAL:HB	2.55	0.41
2:B:61:GLU:HG2	2:B:86:GLU:O	2.21	0.41
2:B:221(A):ARG:HD2	6:D:454:HOH:O	2.21	0.41
2:D:61:GLU:HG2	2:D:86:GLU:O	2.20	0.41
2:D:31:VAL:HB	2:D:44:ALA:HB3	2.03	0.41
2:D:75:ARG:HD2	6:D:445:HOH:O	2.21	0.40
2:D:242:ILE:O	2:D:245:PHE:CE1	2.73	0.40
2:D:28:PRO:HG2	2:D:29:TRP:CE3	2.57	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	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
1	C	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
2	B	238/257 (93%)	232 (98%)	6 (2%)	0	100	100
2	D	239/257 (93%)	222 (93%)	14 (6%)	3 (1%)	9	3
All	All	531/574 (92%)	506 (95%)	22 (4%)	3 (1%)	21	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	186(B)	GLU
2	D	186(C)	GLY
2	D	171	SER

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	27/27 (100%)	27 (100%)	0	100	100
1	C	26/27 (96%)	26 (100%)	0	100	100
2	B	211/223 (95%)	206 (98%)	5 (2%)	43	38
2	D	215/223 (96%)	208 (97%)	7 (3%)	33	26
All	All	479/500 (96%)	467 (98%)	12 (2%)	42	37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	75	ARG
2	B	154	VAL
2	B	180	MET
2	B	205	ASN
2	B	240	LYS

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Mol	Chain	Res	Type
2	D	50	ARG
2	D	65	LEU
2	D	131	GLN
2	D	173	ARG
2	D	182	CYS
2	D	224	LYS
2	D	236	LYS

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

Mol	Chain	Res	Type
2	B	131	GLN
2	B	204(B)	ASN
2	B	205	ASN
2	B	209	GLN
2	D	71	HIS
2	D	95	ASN
2	D	204(B)	ASN
2	D	209	GLN
2	D	239	GLN

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDG	B	401	-	15,15,15	0.40	0	21,21,21	0.67	0

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	NDG	B	401	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NDG	C8-C7-N2-C2
3	B	401	NDG	O7-C7-N2-C2
3	B	401	NDG	C4-C5-C6-O6
3	B	401	NDG	O5-C5-C6-O6

There are no ring outliers.

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

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	30/30 (100%)	0.34	3 (10%) 12 13	20, 28, 44, 59	0
1	C	28/30 (93%)	0.76	5 (17%) 3 3	24, 34, 50, 73	0
2	B	242/257 (94%)	0.01	8 (3%) 49 52	16, 26, 42, 61	0
2	D	245/257 (95%)	0.65	31 (12%) 8 8	18, 33, 66, 82	0
All	All	545/574 (94%)	0.36	47 (8%) 16 17	16, 30, 60, 82	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	245	PHE	4.7
2	D	191	CYS	4.6
1	A	1(B)	ALA	4.2
2	D	186(C)	GLY	4.2
2	D	173	ARG	4.1
2	B	245	PHE	4.1
2	D	168	CYS	4.1
2	D	186	PRO	3.7
2	D	220	CYS	3.3
2	D	215	TRP	3.3
2	D	172	THR	3.2
2	B	60(E)	ASP	3.1
1	C	14(K)	ILE	3.0
2	D	60(D)	TRP	3.0
2	D	176	ILE	3.0
2	B	60(D)	TRP	3.0
2	D	193	GLY	2.9
2	D	186(A)	ASP	2.9
2	D	216	GLY	2.9
2	D	96	TRP	2.8
2	D	92	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	142	GLY	2.8
2	D	169	LYS	2.8
2	D	151	GLN	2.7
2	D	174	ILE	2.7
2	D	219	GLY	2.6
2	D	143	ASN	2.6
1	C	14(L)	ASP	2.6
2	D	167	VAL	2.6
1	C	1(B)	ALA	2.6
2	D	97(A)	GLU	2.5
1	A	14(N)	ARG	2.5
2	D	60(C)	PRO	2.5
2	D	60(A)	TYR	2.5
2	D	60(G)	ASN	2.4
2	B	204(A)	PHE	2.4
2	D	170	ASP	2.4
2	B	78	ASN	2.4
2	B	36(A)	SER	2.2
2	D	227	PHE	2.2
1	A	1(A)	ASP	2.1
2	D	171	SER	2.1
2	D	186(B)	GLU	2.1
1	C	12	LEU	2.1
2	D	99	LEU	2.1
1	C	14(H)	GLU	2.0
2	B	75	ARG	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($\text{\AA}^2$)	Q<0.9
3	NDG	B	401	15/15	0.74	0.19	79,83,85,86	0
4	K	B	403	1/1	0.98	0.06	35,35,35,35	0
4	K	D	404	1/1	0.99	0.05	33,33,33,33	0
5	CL	D	402	1/1	0.99	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.