Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 11:36 AM EDT

PDB ID	:	1ZR0
Title	:	Crystal Structure of Kunitz Domain 1 of Tissue Factor Pathway Inhibitor-2 with Bovine Trypsin
Authors	:	Schmidt, A.E.; Chand, H.S.; Cascio, D.; Kisiel, W.; Bajaj, S.P.
Deposited on	:	2005-05-18
Resolution	:	1.80 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:

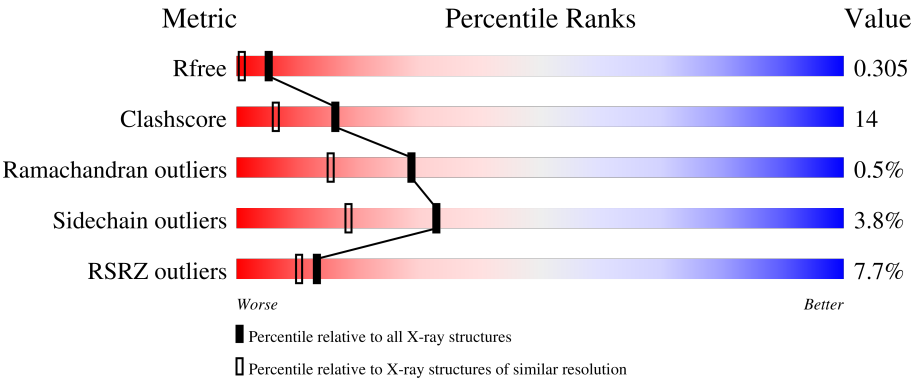
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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 <=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	223	88% 10% ·
1	C	223	18% 60% 32% 6% ·
2	B	63	2% 78% 19% ·
2	D	63	2% 92% 5% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4809 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1628	1012	279	323	14			
1	C	223	Total	C	N	O	S	0	0	0
			1628	1012	279	323	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	THR	ASP	conflict	UNP P00760
C	98	THR	ASP	conflict	UNP P00760

- Molecule 2 is a protein called Tissue factor pathway inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	63	Total	C	N	O	S	0	0	0
			516	326	87	97	6			
2	D	63	Total	C	N	O	S	0	0	0
			516	326	87	97	6			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total	O	0	0
			242	242		

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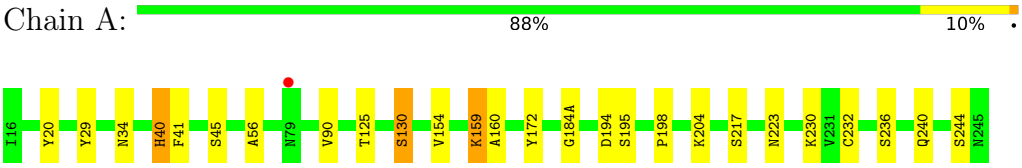
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	77	Total O 77 77	0	0
4	C	123	Total O 123 123	0	0
4	D	77	Total O 77 77	0	0

3 Residue-property plots (i)

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

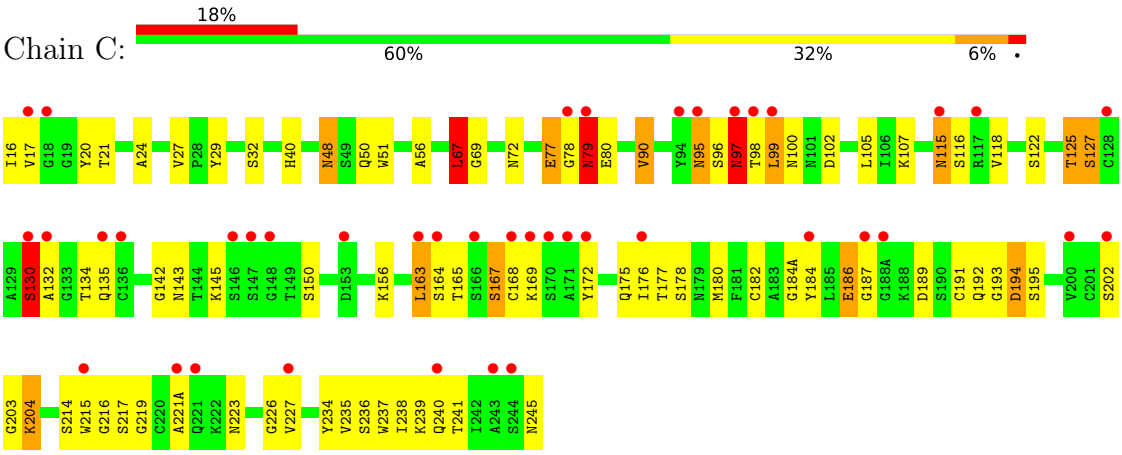
• Molecule 1: Cationic trypsin

Chain A:



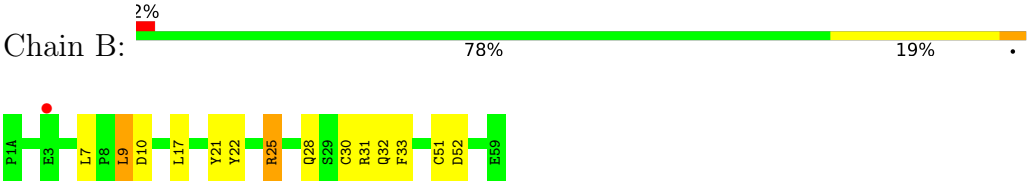
• Molecule 1: Cationic trypsin

Chain C:



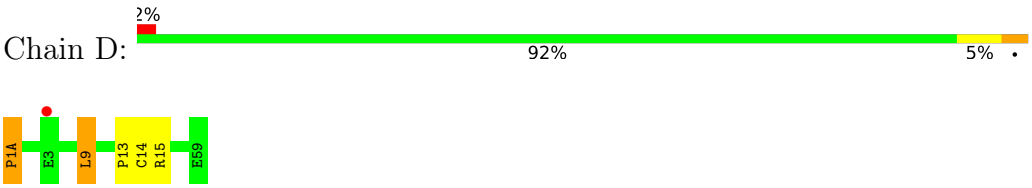
• Molecule 2: Tissue factor pathway inhibitor 2

Chain B:



• Molecule 2: Tissue factor pathway inhibitor 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.11Å 77.01Å 125.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 9.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (10.00-1.80) 95.1 (9.82-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.231 , 0.295 0.244 , 0.305	Depositor DCC
R_{free} test set	3188 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4809	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA

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	1.28	8/1659 (0.5%)	1.04	3/2249 (0.1%)
1	C	1.38	5/1657 (0.3%)	1.16	9/2243 (0.4%)
2	B	1.26	0/531	1.30	8/722 (1.1%)
2	D	1.28	1/531 (0.2%)	1.11	2/722 (0.3%)
All	All	1.32	14/4378 (0.3%)	1.13	22/5936 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	LEU	C-N	24.28	1.76	1.33
1	C	125	THR	C-N	15.83	1.70	1.34
1	C	204	LYS	C-N	14.40	1.67	1.34
1	A	130	SER	C-N	12.31	1.62	1.34
1	A	217	SER	C-N	7.56	1.46	1.33
1	A	125	THR	C-N	7.13	1.50	1.34
1	C	72	ASN	C-O	7.05	1.36	1.23
1	A	195	SER	CB-OG	-6.62	1.33	1.42
1	A	34	ASN	C-N	6.48	1.49	1.34
1	A	172	TYR	CE1-CZ	-6.46	1.30	1.38
1	A	154	VAL	CB-CG1	5.75	1.65	1.52
1	C	130	SER	C-O	5.20	1.33	1.23
1	A	29	TYR	CD2-CE2	-5.01	1.31	1.39
2	D	1(A)	PRO	N-CA	5.00	1.55	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	THR	O-C-N	-15.22	98.35	122.70
1	C	67	LEU	C-N-CA	-10.17	100.95	122.30
1	C	67	LEU	O-C-N	9.26	138.94	123.20
1	A	125	THR	C-N-CA	8.59	143.17	121.70
2	B	10	ASP	CB-CG-OD2	8.58	126.02	118.30
1	A	125	THR	O-C-N	-7.77	110.27	122.70
1	C	204	LYS	C-N-CA	-7.49	102.99	121.70
2	B	31	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	D	9	LEU	CA-CB-CG	7.24	131.94	115.30
2	B	9	LEU	CB-CG-CD1	-7.03	99.05	111.00
2	D	9	LEU	CB-CG-CD2	6.97	122.84	111.00
1	C	67	LEU	CA-C-N	-6.63	102.93	116.20
2	B	52	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	194	ASP	CB-CG-OD2	6.26	123.94	118.30
2	B	31	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	194	ASP	CB-CG-OD2	6.13	123.82	118.30
2	B	7	LEU	CA-CB-CG	5.83	128.71	115.30
2	B	25	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	97	ASN	CB-CA-C	5.47	121.33	110.40
1	C	100	ASN	N-CA-C	-5.06	97.35	111.00
2	B	17	LEU	CB-CG-CD2	5.05	119.58	111.00
1	C	90	VAL	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	SER	Mainchain
1	A	204	LYS	Mainchain
1	A	40	HIS	Sidechain

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	1628	0	1593	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1628	0	1589	97	0
2	B	516	0	468	6	0
2	D	516	0	464	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	242	0	0	2	0
4	B	77	0	0	1	0
4	C	123	0	0	9	0
4	D	77	0	0	1	0
All	All	4809	0	4114	118	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 14.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:C	1:C:127:SER:N	1.70	1.45
1:C:67:LEU:C	1:C:69:GLY:N	1.76	1.38
1:C:217:SER:C	1:C:219:GLY:N	2.20	0.95
2:B:30:CYS:HG	2:B:51:CYS:HG	1.09	0.91
1:C:177:THR:HG22	1:C:178:SER:H	1.38	0.88
1:C:96:SER:O	1:C:97:ASN:ND2	2.05	0.87
1:C:130:SER:C	1:C:132:ALA:N	2.28	0.86
1:C:17:VAL:HG21	1:C:221(A):ALA:HB2	1.56	0.85
1:C:115:ASN:HD22	1:C:115:ASN:N	1.74	0.85
1:C:187:GLY:HA2	4:C:1056:HOH:O	1.76	0.83
1:A:240:GLN:HG3	4:C:1043:HOH:O	1.79	0.82
1:C:180:MET:CE	1:C:227:VAL:HG11	2.10	0.81
1:C:24:ALA:HB1	4:C:1062:HOH:O	1.80	0.80
1:C:67:LEU:C	1:C:69:GLY:CA	2.50	0.80
1:C:143:ASN:HB3	1:C:191:CYS:SG	2.22	0.78
1:C:77:GLU:OE1	1:C:78:GLY:O	2.02	0.77
1:C:115:ASN:CG	4:C:1119:HOH:O	2.25	0.74
1:C:98:THR:O	1:C:99:LEU:HG	1.89	0.72
1:C:95:ASN:ND2	1:C:96:SER:O	2.24	0.71
1:C:202:SER:O	1:C:202:SER:OG	2.07	0.70
1:C:180:MET:HE3	1:C:227:VAL:HG11	1.73	0.70
1:C:176:ILE:HD13	1:C:180:MET:CE	2.23	0.69
1:C:78:GLY:O	1:C:79:ASN:HB3	1.94	0.67
1:A:40:HIS:C	1:A:40:HIS:CD2	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:N	1:C:194:ASP:OD2	2.28	0.67
1:C:67:LEU:CA	1:C:69:GLY:N	2.58	0.67
1:C:177:THR:HG22	1:C:178:SER:N	2.09	0.67
1:C:204:LYS:NZ	4:C:1012:HOH:O	2.28	0.66
1:C:125:THR:O	1:C:127:SER:N	2.25	0.66
1:C:164:SER:HB3	1:C:167:SER:OG	1.97	0.65
1:C:17:VAL:CG2	1:C:221(A):ALA:HB2	2.28	0.64
1:C:163:LEU:HD22	1:C:182:CYS:HB2	1.79	0.64
1:C:176:ILE:HD13	1:C:180:MET:HE1	1.80	0.64
1:A:230:LYS:NZ	4:A:1227:HOH:O	2.29	0.63
1:C:163:LEU:HD22	1:C:182:CYS:CB	2.29	0.63
1:C:180:MET:HE3	1:C:227:VAL:CG1	2.27	0.62
1:C:217:SER:C	1:C:219:GLY:CA	2.67	0.62
1:C:96:SER:OG	1:C:97:ASN:N	2.31	0.62
1:A:20:TYR:OH	1:A:159:LYS:HE2	2.00	0.62
1:C:99:LEU:HD21	1:C:215:TRP:CD1	2.34	0.62
1:C:125:THR:CA	1:C:127:SER:N	2.63	0.60
2:B:28:GLN:NE2	4:B:100:HOH:O	2.35	0.60
1:C:99:LEU:CD2	1:C:215:TRP:CD1	2.85	0.60
1:C:48:ASN:HB3	1:C:50:GLN:H	1.67	0.59
1:C:99:LEU:HG	1:C:99:LEU:O	2.04	0.58
1:C:115:ASN:N	1:C:115:ASN:ND2	2.48	0.58
1:C:241:THR:HA	1:C:245:ASN:ND2	2.18	0.57
1:C:21:THR:OG1	1:C:156:LYS:NZ	2.22	0.57
1:C:99:LEU:HD21	1:C:215:TRP:NE1	2.20	0.56
2:B:21:TYR:CE2	2:B:32:GLN:HG3	2.41	0.56
1:C:241:THR:HA	1:C:245:ASN:HD22	1.70	0.56
1:C:115:ASN:HD21	1:C:118:VAL:HB	1.70	0.55
1:C:99:LEU:HD11	1:C:215:TRP:HE1	1.71	0.55
1:A:236:SER:O	1:A:240:GLN:HG2	2.06	0.54
1:C:172:TYR:HB3	1:C:175:GLN:HE21	1.72	0.54
1:C:98:THR:O	1:C:99:LEU:O	2.25	0.54
2:B:9:LEU:HD11	2:B:33:PHE:CG	2.42	0.54
1:C:115:ASN:ND2	1:C:118:VAL:HB	2.23	0.53
1:C:17:VAL:HG13	1:C:191:CYS:SG	2.49	0.53
1:C:176:ILE:HD13	1:C:180:MET:HE2	1.89	0.53
1:C:236:SER:O	1:C:240:GLN:HG3	2.08	0.53
1:C:99:LEU:O	1:C:99:LEU:CG	2.57	0.52
1:C:99:LEU:HD11	1:C:215:TRP:NE1	2.24	0.52
1:C:165:THR:HG21	4:C:1071:HOH:O	2.09	0.51
1:C:56:ALA:N	1:C:102:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:HIS:HE1	1:C:193:GLY:O	1.93	0.50
1:C:95:ASN:HD22	1:C:95:ASN:C	2.13	0.50
1:A:40:HIS:C	1:A:40:HIS:HD2	2.15	0.50
1:C:192:GLN:NE2	2:D:14:CYS:O	2.40	0.50
1:C:165:THR:HG22	1:C:169:LYS:HE3	1.94	0.49
2:D:1(A):PRO:HD3	4:D:129:HOH:O	2.12	0.49
2:B:9:LEU:HD13	2:B:22:TYR:CG	2.47	0.49
1:C:105:LEU:HD12	1:C:237:TRP:CH2	2.48	0.49
1:C:177:THR:CG2	1:C:178:SER:N	2.76	0.49
1:C:214:SER:HB3	1:C:227:VAL:O	2.13	0.49
1:C:241:THR:HG23	1:C:245:ASN:ND2	2.28	0.49
1:C:130:SER:O	1:C:132:ALA:C	2.52	0.48
1:C:184:TYR:HB3	1:C:186:GLU:HG3	1.95	0.48
1:C:105:LEU:HD12	1:C:237:TRP:CZ3	2.49	0.48
1:C:236:SER:O	1:C:240:GLN:CG	2.62	0.47
1:A:20:TYR:OH	1:A:159:LYS:CE	2.62	0.47
1:A:40:HIS:HD2	1:A:41:PHE:N	2.12	0.47
1:C:145:LYS:HE3	1:C:150:SER:HB2	1.96	0.47
1:C:184:TYR:HB3	1:C:186:GLU:CG	2.44	0.47
1:C:122:SER:OG	1:C:203:GLY:O	2.32	0.47
1:A:45:SER:OG	1:A:198:PRO:HB3	2.15	0.47
1:C:180:MET:HE1	1:C:215:TRP:CZ2	2.50	0.46
1:C:99:LEU:HD21	1:C:215:TRP:CE2	2.49	0.46
1:C:234:TYR:O	1:C:238:ILE:HG13	2.15	0.46
1:C:95:ASN:HD21	1:C:97:ASN:ND2	2.13	0.46
1:C:78:GLY:O	1:C:79:ASN:CB	2.63	0.45
1:C:195:SER:OG	2:D:15:ARG:C	2.54	0.45
1:A:244:SER:HB3	1:C:223:ASN:HD21	1.82	0.45
2:B:9:LEU:HD12	2:B:9:LEU:HA	1.77	0.44
1:C:56:ALA:HB1	1:C:90:VAL:HG13	1.98	0.44
1:C:145:LYS:HE3	1:C:150:SER:CB	2.47	0.44
1:A:223:ASN:HB3	4:A:1091:HOH:O	2.17	0.44
1:A:230:LYS:HE3	1:A:232:CYS:SG	2.58	0.44
1:A:56:ALA:HB1	1:A:90:VAL:HG13	1.99	0.44
1:C:172:TYR:HB3	1:C:175:GLN:NE2	2.34	0.43
1:C:235:VAL:O	1:C:239:LYS:HG2	2.19	0.42
1:C:180:MET:CE	1:C:227:VAL:CG1	2.86	0.42
1:C:17:VAL:HG22	1:C:189:ASP:O	2.20	0.42
1:C:216:GLY:O	2:D:13:PRO:CB	2.67	0.42
1:C:184(A):GLY:C	1:C:184:TYR:CD1	2.93	0.42
1:C:168:CYS:SG	1:C:176:ILE:HD12	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:CD	1:C:79:ASN:HD22	2.23	0.41
1:C:48:ASN:HB2	1:C:51:TRP:HB2	2.01	0.41
1:C:142:GLY:HA2	1:C:193:GLY:HA3	2.02	0.41
1:C:27:VAL:HG13	1:C:29:TYR:CZ	2.55	0.41
1:A:160:ALA:HB1	1:A:184(A):GLY:HA2	2.03	0.41
1:C:20:TYR:HA	4:C:1096:HOH:O	2.20	0.41
1:C:32:SER:OG	1:C:40:HIS:HD2	2.03	0.41
1:C:182:CYS:HA	1:C:226:GLY:O	2.21	0.41
1:C:217:SER:O	4:C:1092:HOH:O	2.20	0.41
1:C:51:TRP:CZ2	1:C:107:LYS:HD3	2.56	0.40
1:A:40:HIS:CD2	1:A:41:PHE:N	2.88	0.40
1:C:236:SER:HB3	4:C:1020:HOH:O	2.21	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	221/223 (99%)	216 (98%)	5 (2%)	0	100 100
1	C	217/223 (97%)	199 (92%)	15 (7%)	3 (1%)	11 3
2	B	61/63 (97%)	58 (95%)	3 (5%)	0	100 100
2	D	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
All	All	560/572 (98%)	530 (95%)	27 (5%)	3 (0%)	29 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	79	ASN
1	C	99	LEU
1	C	80	GLU

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	184/184 (100%)	183 (100%)	1 (0%)	88 87
1	C	184/184 (100%)	169 (92%)	15 (8%)	11 3
2	B	53/53 (100%)	52 (98%)	1 (2%)	57 46
2	D	53/53 (100%)	52 (98%)	1 (2%)	57 46
All	All	474/474 (100%)	456 (96%)	18 (4%)	33 18

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
2	B	25	ARG
1	C	48	ASN
1	C	67	LEU
1	C	77	GLU
1	C	79	ASN
1	C	95	ASN
1	C	97	ASN
1	C	115	ASN
1	C	116	SER
1	C	127	SER
1	C	130	SER
1	C	134	THR
1	C	135	GLN
1	C	163	LEU
1	C	167	SER
1	C	186	GLU
2	D	9	LEU

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	91	HIS

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Mol	Chain	Res	Type
1	A	223	ASN
2	B	32	GLN
1	C	40	HIS
1	C	50	GLN
1	C	95	ASN
1	C	115	ASN
1	C	175	GLN
1	C	223	ASN
1	C	245	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	5
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	130:SER	C	132:ALA	N	2.28
1	C	217:SER	C	219:GLY	N	2.20
1	C	67:LEU	C	69:GLY	N	1.76
1	C	125:THR	C	127:SER	N	1.70
1	C	204:LYS	C	209:LEU	N	1.67
1	A	130:SER	C	132:ALA	N	1.62

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, 95^{th} 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	223/223 (100%)	-0.13	1 (0%) 92 90	20, 31, 42, 49	0
1	C	223/223 (100%)	0.99	41 (18%) 1 0	22, 47, 59, 66	0
2	B	63/63 (100%)	-0.05	1 (1%) 72 68	20, 28, 39, 44	1 (1%)
2	D	63/63 (100%)	0.09	1 (1%) 72 68	25, 31, 42, 47	1 (1%)
All	All	572/572 (100%)	0.34	44 (7%) 13 10	20, 34, 56, 66	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	SER	6.3
1	C	188(A)	GLY	4.7
1	C	243	ALA	4.4
1	C	170	SER	4.0
1	C	128	CYS	3.7
1	C	187	GLY	3.7
1	C	244	SER	3.6
1	C	148	GLY	3.6
1	C	130	SER	3.5
1	C	163	LEU	3.4
2	B	3	GLU	3.3
1	C	164	SER	3.3
1	C	147	SER	3.0
1	C	78	GLY	3.0
1	C	99	LEU	3.0
2	D	3	GLU	2.8
1	C	168	CYS	2.8
1	C	97	ASN	2.8
1	C	18	GLY	2.7
1	C	95	ASN	2.7
1	C	176	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	184	TYR	2.7
1	C	115	ASN	2.6
1	C	146	SER	2.6
1	C	117	ARG	2.6
1	C	240	GLN	2.6
1	C	132	ALA	2.5
1	C	153	ASP	2.5
1	C	227	VAL	2.5
1	C	79	ASN	2.5
1	C	221	GLN	2.4
1	C	135	GLN	2.4
1	C	94	TYR	2.4
1	C	202	SER	2.3
1	C	17	VAL	2.3
1	C	136	CYS	2.3
1	C	215	TRP	2.3
1	C	221(A)	ALA	2.2
1	C	169	LYS	2.1
1	C	98	THR	2.1
1	C	200	VAL	2.0
1	C	171	ALA	2.0
1	A	79	ASN	2.0
1	C	172	TYR	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 monosaccharides 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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	1002	1/1	0.93	0.07	38,38,38,38	0
3	CA	A	1001	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.