Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 AM GMT

PDB ID	:	2QYI
Title	:	Crystal structure of a binary complex between an engineered trypsin inhibitor and Bovine trypsin
Authors	:	Khamrui, S.; Dasgupta, J.; Dattagupta, J.K.; Sen, U.
Deposited on	:	2007-08-15
Resolution	:	2.60 Å(reported)

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

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

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the ⓘ symbol.

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

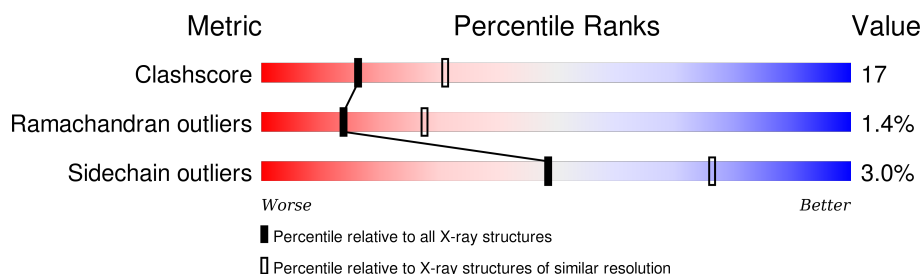|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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
Clashscore		17
Ramachandran outliers		1.4%
Sidechain outliers		3.0%

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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	223	70% 27% •
1	C	223	70% 28% •
2	B	183	62% 32% • •
2	D	183	66% 28% •• •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6315 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			

- Molecule 2 is a protein called Chymotrypsin inhibitor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1372	870	239	259	4			
2	D	175	Total	C	N	O	S	0	0	0
			1372	870	239	259	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	668	ARG	LEU	ENGINEERED	UNP P10822
D	868	ARG	LEU	ENGINEERED	UNP P10822

- 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 NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		

• Molecule 5 is water.

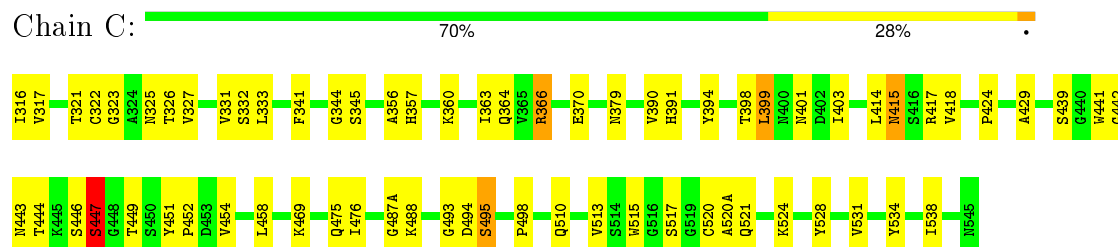| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	61	Total 61	O 61	0	0
5	C	85	Total 85	O 85	0	0
5	D	78	Total 78	O 78	0	0

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.
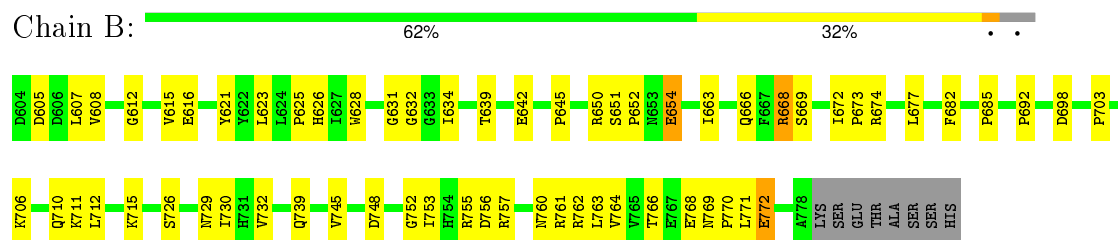
Note EDS was not executed.

- Molecule 1: Cationic trypsin

Chain A:

- Molecule 1: Cationic trypsin

Chain C:

- Molecule 2: Chymotrypsin inhibitor 3

Chain B:

- Molecule 2: Chymotrypsin inhibitor 3

Chain D:
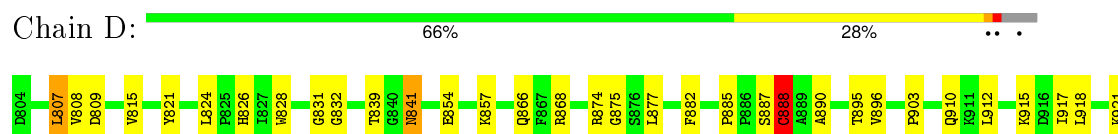
F922 E923 K924 V925 S926 N929 Y933 Y937 E942 E943 D944 V945 K946 C947 D948 Q949 R961 R962 V965 T966 E967 E968 N969 P970 L971 E972 L975 A978 LYS SER GLU THR ALA SER SER HIS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.69Å 77.44Å 72.91Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.3 (20.00-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6315	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.37	0/1659	0.66	0/2250
1	C	0.36	0/1659	0.68	1/2250 (0.0%)
2	B	0.36	0/1406	0.72	0/1914
2	D	0.36	0/1406	0.73	0/1914
All	All	0.36	0/6130	0.70	1/8328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	447	SER	N-CA-C	-5.82	95.28	111.00

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	1628	0	1588	52	0
1	C	1628	0	1588	61	0
2	B	1372	0	1349	53	0
2	D	1372	0	1349	47	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	88	0	0	7	0
5	B	61	0	0	7	0
5	C	85	0	0	2	0
5	D	78	0	0	6	0
All	All	6315	0	5874	198	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 17.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:HB3	2:B:745:VAL:HG13	1.53	0.91
1:A:48:ASN:ND2	1:A:50:GLN:H	1.77	0.83
2:B:605:ASP:HB2	2:B:674:ARG:HB3	1.61	0.82
2:D:887:SER:O	2:D:888:CYS:HB3	1.79	0.80
1:C:325:ASN:ND2	1:C:417:ARG:HD2	1.98	0.79
2:B:753:ILE:HD11	2:B:771:LEU:HD21	1.66	0.78
1:C:475:GLN:HE22	2:D:866:GLN:HE22	1.31	0.78
1:C:517:SER:HB2	1:C:524:LYS:HD2	1.67	0.76
1:C:495:SER:HB2	2:D:868:ARG:O	1.86	0.76
1:C:446:SER:CB	1:C:520:CYS:HB2	2.16	0.75
1:C:446:SER:HB3	1:C:520:CYS:HB2	1.70	0.72
1:C:323:GLY:O	1:C:326:THR:HG22	1.89	0.72
1:C:345:SER:OG	1:C:498:PRO:HB3	1.90	0.71
2:D:944:ASP:HB2	5:D:1127:HOH:O	1.91	0.70
2:B:639:THR:HB	2:B:762:ARG:HH21	1.57	0.68
1:A:45:SER:OG	1:A:198:PRO:HB3	1.94	0.67
1:C:326:THR:HG23	1:C:327:VAL:HG23	1.77	0.67
1:A:215:TRP:HA	2:B:668:ARG:HG2	1.77	0.65
1:C:417:ARG:HH11	1:C:417:ARG:HG3	1.61	0.65
2:B:685:PRO:HG3	2:B:692:PRO:HB3	1.79	0.65
2:D:877:LEU:HD11	2:D:945:VAL:HG11	1.77	0.64
1:A:97:ASN:HB3	2:B:745:VAL:CG1	2.27	0.62
1:C:316:ILE:O	1:C:444:THR:HA	2.00	0.62
2:D:946:LYS:NZ	2:D:948:ASP:HB3	2.14	0.61
1:C:322:CYS:HB3	1:C:326:THR:HG21	1.81	0.61
1:C:475:GLN:NE2	2:D:866:GLN:HE22	1.98	0.61
2:D:875:GLY:HA2	2:D:921:LYS:HE3	1.83	0.61
1:C:469:LYS:HG2	1:C:476:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:VAL:HG22	1:C:444:THR:C	2.21	0.60
1:C:449:THR:HG23	1:C:451:TYR:HE1	1.66	0.60
2:D:896:VAL:HG21	2:D:937:TYR:CD1	2.37	0.59
1:C:449:THR:HG23	1:C:451:TYR:CE1	2.38	0.58
1:A:213:VAL:HA	1:A:228:TYR:CD2	2.38	0.58
2:B:650:ARG:NH1	5:B:1222:HOH:O	2.36	0.58
1:C:317:VAL:HG22	1:C:444:THR:O	2.04	0.58
2:B:732:VAL:HG11	2:B:772:GLU:HG2	1.86	0.58
1:C:444:THR:HG23	1:C:452:PRO:HD3	1.85	0.58
1:A:114:LEU:HD23	1:A:119:ALA:HA	1.86	0.58
2:B:756:ASP:OD2	2:B:760:ASN:HB2	2.04	0.57
1:C:424:PRO:HB3	1:C:510:GLN:OE1	2.04	0.57
1:C:458:LEU:HD11	1:C:488:LYS:HB3	1.87	0.57
2:B:753:ILE:HA	2:B:762:ARG:O	2.05	0.56
1:C:325:ASN:CG	1:C:417:ARG:HD2	2.25	0.56
2:D:917:ILE:HG13	2:D:918:LEU:HD13	1.88	0.56
2:D:946:LYS:HD2	5:D:1253:HOH:O	2.04	0.56
1:A:48:ASN:OD1	1:A:51:TRP:HB2	2.06	0.56
1:A:124:PRO:HD3	1:A:209:LEU:O	2.06	0.56
1:A:72:ASN:HA	1:A:153:ASP:O	2.06	0.55
1:C:415:ASN:HD22	1:C:418:VAL:H	1.54	0.55
1:A:94:TYR:HA	1:A:101:ASN:HB2	1.88	0.55
1:A:186:GLU:HG2	1:A:186:GLU:O	2.05	0.55
1:C:317:VAL:O	1:C:488:LYS:HA	2.07	0.55
2:D:826:HIS:HE1	2:D:972:GLU:OE2	1.90	0.55
2:B:764:VAL:HG23	2:B:766:THR:HG23	1.89	0.55
2:D:826:HIS:HD2	2:D:828:TRP:H	1.53	0.54
2:D:841:ASN:HD22	2:D:841:ASN:N	2.04	0.54
2:D:915:LYS:HE3	5:D:1160:HOH:O	2.08	0.53
1:C:398:THR:C	1:C:399:LEU:HD12	2.29	0.53
1:C:521:GLN:HB2	1:C:524:LYS:HB2	1.89	0.53
2:B:625:PRO:HB3	2:B:650:ARG:CZ	2.38	0.53
1:C:357:HIS:NE2	1:C:495:SER:OG	2.36	0.52
1:A:17:VAL:HG22	1:A:144:THR:C	2.29	0.52
1:A:213:VAL:HA	1:A:228:TYR:HD2	1.73	0.52
2:D:841:ASN:HD22	2:D:841:ASN:H	1.57	0.52
2:B:663:ILE:HG22	2:B:672:ILE:CD1	2.39	0.52
1:C:322:CYS:HB3	1:C:326:THR:CG2	2.39	0.52
2:B:710:GLN:O	2:B:712:LEU:HD13	2.10	0.52
1:C:364:GLN:OE1	1:C:366:ARG:NH1	2.33	0.52
2:B:682:PHE:O	2:B:685:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:ASP:HB3	5:B:1156:HOH:O	2.08	0.51
2:B:628:TRP:CE3	2:B:654:GLU:O	2.64	0.51
1:A:114:LEU:HD23	1:A:118:VAL:O	2.10	0.51
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.92	0.51
1:C:356:ALA:HB1	1:C:390:VAL:HG13	1.93	0.51
1:C:513:VAL:HA	1:C:528:TYR:CD2	2.46	0.51
1:A:213:VAL:HG22	1:A:228:TYR:HE2	1.76	0.50
2:B:639:THR:HB	2:B:762:ARG:NH2	2.25	0.50
1:C:415:ASN:ND2	1:C:418:VAL:H	2.09	0.50
1:A:236:SER:O	1:A:240:GLN:HG3	2.11	0.50
1:C:534:TYR:O	1:C:538:ILE:HG13	2.12	0.49
2:B:755:ARG:HH22	2:B:761:ARG:NH1	2.10	0.49
1:A:64:GLN:NE2	1:A:82:PHE:HB3	2.27	0.49
2:B:605:ASP:HA	2:B:674:ARG:HH21	1.77	0.49
1:C:417:ARG:NH1	1:C:417:ARG:HG3	2.25	0.49
2:B:755:ARG:NH2	2:B:761:ARG:NH1	2.60	0.49
1:A:215:TRP:CE2	1:A:227:VAL:HG11	2.48	0.49
2:B:615:VAL:HG13	2:B:621:TYR:CZ	2.47	0.49
1:A:215:TRP:CZ2	1:A:227:VAL:HG11	2.47	0.49
2:D:841:ASN:H	2:D:841:ASN:ND2	2.10	0.49
1:A:114:LEU:CD2	1:A:119:ALA:HA	2.42	0.49
2:D:966:THR:HG22	2:D:968:GLU:H	1.78	0.48
1:A:98:THR:C	1:A:99:LEU:HD12	2.33	0.48
1:C:442:GLY:HA2	1:C:493:GLY:HA3	1.93	0.48
1:C:487(A):GLY:H	1:C:520(A):ALA:HB1	1.78	0.48
1:A:54:SER:OG	1:A:196:GLY:HA3	2.14	0.47
1:A:64:GLN:HE21	1:A:82:PHE:HB3	1.78	0.47
1:A:39:TYR:HB3	5:A:1029:HOH:O	2.14	0.47
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.79	0.47
2:B:663:ILE:HG22	2:B:672:ILE:HD11	1.96	0.47
2:B:768:GLU:OE2	2:B:768:GLU:HA	2.15	0.47
1:C:370:GLU:HB2	5:C:1077:HOH:O	2.14	0.47
5:A:1026:HOH:O	2:B:668:ARG:HD3	2.13	0.47
1:C:332:SER:HB2	1:C:441:TRP:CZ3	2.50	0.47
1:C:316:ILE:CD1	1:C:439:SER:HA	2.45	0.47
2:B:632:GLY:O	2:B:650:ARG:HG3	2.14	0.47
2:B:715:LYS:HD3	5:B:1141:HOH:O	2.15	0.47
2:D:809:ASP:HB2	2:D:975:LEU:O	2.14	0.47
2:B:628:TRP:HE3	2:B:654:GLU:O	1.98	0.47
1:A:219:GLY:O	2:B:668:ARG:NH1	2.48	0.46
2:B:732:VAL:HG11	2:B:772:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:HD12	5:C:1294:HOH:O	2.14	0.46
2:B:769:ASN:N	2:B:770:PRO:CD	2.78	0.46
1:A:29:TYR:CZ	1:A:200:VAL:HG21	2.51	0.46
1:C:331:VAL:HG22	1:C:344:GLY:C	2.35	0.46
2:D:917:ILE:HG13	2:D:918:LEU:CD1	2.45	0.46
2:D:948:ASP:O	2:D:949:GLN:HG3	2.16	0.46
1:C:446:SER:O	1:C:447:SER:HB2	2.15	0.46
2:B:615:VAL:HG13	2:B:621:TYR:CE1	2.51	0.46
2:B:677:LEU:HD11	2:B:745:VAL:HG21	1.98	0.46
1:C:515:TRP:HA	2:D:868:ARG:HG3	1.96	0.46
2:D:946:LYS:HZ1	2:D:948:ASP:HB3	1.79	0.46
2:B:710:GLN:HE21	2:D:910:GLN:HE21	1.63	0.46
1:A:145:LYS:HE3	1:A:150:SER:HB2	1.97	0.46
2:B:739:GLN:HG2	5:B:1061:HOH:O	2.15	0.46
1:C:394:TYR:HA	1:C:401:ASN:HB2	1.97	0.46
1:A:175:GLN:HE22	2:B:666:GLN:HE22	1.64	0.46
1:A:91:HIS:HB2	1:A:103:ILE:HG23	1.98	0.46
2:D:815:VAL:HG13	2:D:821:TYR:CE1	2.51	0.45
1:A:243:ALA:HA	5:A:1168:HOH:O	2.16	0.45
2:B:757:ARG:HG2	2:B:757:ARG:HH11	1.82	0.45
2:B:625:PRO:HG3	2:B:631:GLY:O	2.17	0.45
1:A:86:SER:HB3	1:A:109:LYS:HB3	1.99	0.45
2:D:961:ARG:NE	5:D:1228:HOH:O	2.46	0.45
1:C:321:THR:HG23	1:C:454:VAL:HG11	1.99	0.45
1:A:117:ARG:HD2	5:A:1149:HOH:O	2.16	0.45
2:D:824:LEU:CD2	2:D:857:LYS:HA	2.47	0.45
2:D:969:ASN:N	2:D:970:PRO:CD	2.80	0.44
2:D:882:PHE:O	2:D:885:PRO:HD3	2.17	0.44
2:B:626:HIS:HB2	2:B:772:GLU:HG2	1.99	0.44
2:B:651:SER:HA	2:B:652:PRO:HD3	1.86	0.44
1:C:357:HIS:CE1	1:C:495:SER:HG	2.29	0.44
2:D:946:LYS:HZ2	2:D:948:ASP:HB3	1.81	0.44
1:A:117:ARG:HG3	5:A:1149:HOH:O	2.17	0.44
2:B:711:LYS:HA	5:B:1164:HOH:O	2.18	0.44
2:B:763:LEU:HG	2:B:771:LEU:HD11	1.99	0.44
1:A:45:SER:HB2	1:A:53:VAL:HG13	2.00	0.44
1:A:191:CYS:O	1:A:194:ASP:HB2	2.17	0.43
2:B:752:GLY:O	2:B:763:LEU:HA	2.18	0.43
2:B:642:GLU:OE2	2:B:706:LYS:NZ	2.50	0.43
1:C:475:GLN:HE22	2:D:866:GLN:NE2	2.06	0.43
2:B:616:GLU:HG3	5:B:1036:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:874:ARG:NH1	5:D:1064:HOH:O	2.51	0.43
1:C:341:PHE:CZ	1:C:360:LYS:HD2	2.53	0.43
2:D:824:LEU:HD21	2:D:857:LYS:HA	2.00	0.43
1:A:101:ASN:HA	1:A:234:TYR:OH	2.19	0.43
1:A:25:ASN:ND2	1:A:117:ARG:HE	2.17	0.43
1:C:321:THR:HG23	1:C:454:VAL:CG1	2.49	0.42
2:D:831:GLY:O	2:D:854:GLU:HA	2.19	0.42
1:C:391:HIS:HB2	1:C:403:ILE:HG23	2.00	0.42
5:A:1134:HOH:O	2:D:887:SER:HB3	2.19	0.42
1:C:443:ASN:HB2	1:C:451:TYR:CZ	2.54	0.42
2:D:839:THR:HB	2:D:962:ARG:NH2	2.35	0.42
1:C:316:ILE:HG13	1:C:494:ASP:OD2	2.19	0.42
1:A:82:PHE:N	1:A:82:PHE:CD1	2.87	0.42
2:D:832:GLY:HA2	5:D:1085:HOH:O	2.20	0.42
2:D:895:THR:HB	2:D:912:LEU:HD13	2.02	0.42
2:D:808:VAL:HG22	2:D:933:TYR:OH	2.19	0.42
2:B:711:LYS:HG3	2:D:890:ALA:HA	2.01	0.41
2:B:623:LEU:HD22	2:B:634:ILE:HD12	2.02	0.41
1:A:192:GLN:HG3	2:B:669:SER:O	2.20	0.41
1:C:379:ASN:ND2	1:C:417:ARG:NH1	2.68	0.41
2:B:672:ILE:HA	2:B:673:PRO:HD3	1.90	0.41
2:B:710:GLN:HE21	2:D:910:GLN:NE2	2.17	0.41
2:B:608:VAL:CG1	2:B:612:GLY:HA2	2.50	0.41
1:C:357:HIS:CE1	1:C:495:SER:OG	2.73	0.41
1:A:115:ASN:OD1	1:A:118:VAL:HB	2.20	0.41
1:A:54:SER:O	1:A:212:ILE:HD13	2.21	0.41
1:A:215:TRP:CH2	1:A:227:VAL:HG21	2.55	0.41
2:D:807:LEU:HD23	2:D:933:TYR:CZ	2.56	0.41
1:A:163:LEU:HD13	1:A:185:LEU:CD2	2.51	0.41
1:C:316:ILE:N	1:C:494:ASP:OD2	2.53	0.41
2:D:841:ASN:ND2	2:D:841:ASN:N	2.67	0.41
2:D:924:LYS:HD3	2:D:933:TYR:CZ	2.56	0.41
1:C:333:LEU:HD22	1:C:363:ILE:HG21	2.03	0.41
1:A:58:CYS:SG	1:A:195:SER:HB3	2.61	0.41
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.56	0.41
2:B:706:LYS:HE2	5:B:1191:HOH:O	2.21	0.41
2:D:923:GLU:O	2:D:933:TYR:HA	2.22	0.41
1:A:59:TYR:HE2	1:A:88:SER:HB2	1.85	0.41
1:C:415:ASN:ND2	1:C:418:VAL:N	2.69	0.40
1:A:105:LEU:HD11	1:A:238:ILE:HA	2.02	0.40
1:C:323:GLY:O	1:C:326:THR:CG2	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ASN:CB	1:C:417:ARG:HD2	2.51	0.40
1:C:398:THR:HG21	2:D:944:ASP:HA	2.02	0.40
1:A:219:GLY:HA2	5:A:1189:HOH:O	2.21	0.40
1:C:429:ALA:HB2	1:C:510:GLN:HG3	2.03	0.40
1:A:16:ILE:O	1:A:144:THR:HG22	2.21	0.40
2:D:903:PRO:HB2	2:D:965:VAL:CG2	2.51	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	221/223 (99%)	202 (91%)	18 (8%)	1 (0%)	34	60
1	C	221/223 (99%)	204 (92%)	15 (7%)	2 (1%)	21	42
2	B	173/183 (94%)	151 (87%)	18 (10%)	4 (2%)	8	14
2	D	173/183 (94%)	152 (88%)	17 (10%)	4 (2%)	8	14
All	All	788/812 (97%)	709 (90%)	68 (9%)	11 (1%)	14	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	730	ILE
1	C	447	SER
2	D	888	CYS
2	D	926	SER
1	A	49	SER
2	D	929	ASN
2	B	645	PRO
2	B	726	SER
2	D	942	GLU

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Mol	Chain	Res	Type
1	C	531	VAL
2	B	703	PRO

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%)	178 (97%)	6 (3%)	45	73
1	C	184/184 (100%)	180 (98%)	4 (2%)	60	83
2	B	153/160 (96%)	147 (96%)	6 (4%)	39	68
2	D	153/160 (96%)	149 (97%)	4 (3%)	54	80
All	All	674/688 (98%)	654 (97%)	20 (3%)	48	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	66	ARG
1	A	99	LEU
1	A	114	LEU
1	A	153	ASP
1	A	186	GLU
2	B	607	LEU
2	B	654	GLU
2	B	668	ARG
2	B	729	ASN
2	B	748	ASP
2	B	772	GLU
1	C	366	ARG
1	C	399	LEU
1	C	415	ASN
1	C	495	SER
2	D	807	LEU
2	D	841	ASN
2	D	888	CYS

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Mol	Chain	Res	Type
2	D	943	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	30	GLN
1	A	48	ASN
1	A	50	GLN
1	A	101	ASN
1	A	175	GLN
1	A	210	GLN
1	A	221	GLN
1	A	223	ASN
1	A	240	GLN
2	B	666	GLN
2	B	729	ASN
2	B	731	HIS
2	B	758	ASN
1	C	325	ASN
1	C	330	GLN
1	C	374	ASN
1	C	379	ASN
1	C	401	ASN
1	C	415	ASN
2	D	826	HIS
2	D	841	ASN
2	D	866	GLN
2	D	884	ASN
2	D	910	GLN
2	D	929	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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 (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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.