



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KZG
Title : DbsCdc42(Y889F)
Authors : Rossman, K.L.; WorthyLake, D.K.; Snyder, J.T.; Siderovski, D.P.; Campbell, S.L.; Sondek, J.
Deposited on : 2002-02-06
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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

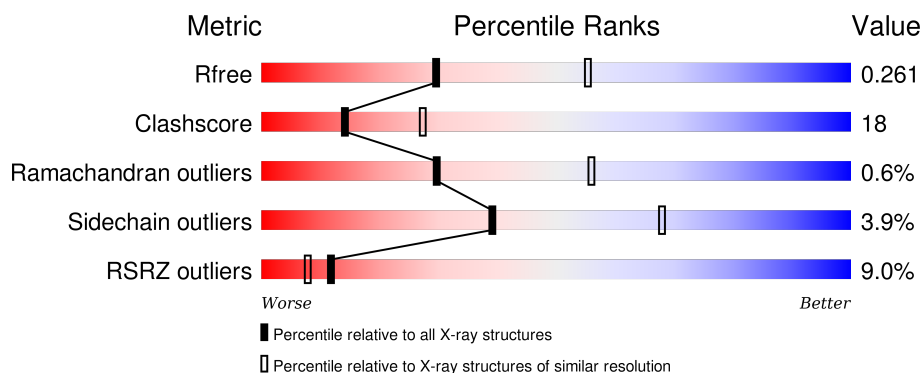
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 $\leq 5\%$. 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	353	<div> <div>6%</div> <div>62%</div> <div>31%</div> <div>5%</div> </div>
1	C	353	<div> <div>12%</div> <div>60%</div> <div>32%</div> <div>7%</div> </div>
2	B	188	<div> <div>6%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
2	D	188	<div> <div>8%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8396 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 GUANINE NUCLEOTIDE EXCHANGE FACTOR DBS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2751	1743	474	513	21			
1	C	330	Total	C	N	O	S	0	0	0
			2680	1702	457	500	21			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	MET	-	INITIATING METHIONINE	UNP Q64096
A	696	ILE	ASN	SEE REMARK 999	UNP Q64096
A	697	PHE	ILE	SEE REMARK 999	UNP Q64096
A	698	LEU	PRO	SEE REMARK 999	UNP Q64096
A	699	ARG	ALA	SEE REMARK 999	UNP Q64096
A	700	GLU	GLY	SEE REMARK 999	UNP Q64096
A	701	LEU	VAL	SEE REMARK 999	UNP Q64096
A	889	PHE	TYR	ENGINEERED	UNP Q64096
A	968	GLU	-	CLONING ARTIFACT	UNP Q64096
A	969	HIS	-	EXPRESSION TAG	UNP Q64096
A	970	HIS	-	EXPRESSION TAG	UNP Q64096
A	971	HIS	-	EXPRESSION TAG	UNP Q64096
A	972	HIS	-	EXPRESSION TAG	UNP Q64096
A	973	HIS	-	EXPRESSION TAG	UNP Q64096
A	974	HIS	-	EXPRESSION TAG	UNP Q64096
C	1622	MET	-	INITIATING METHIONINE	UNP Q64096
C	1696	ILE	ASN	SEE REMARK 999	UNP Q64096
C	1697	PHE	ILE	SEE REMARK 999	UNP Q64096
C	1698	LEU	PRO	SEE REMARK 999	UNP Q64096
C	1699	ARG	ALA	SEE REMARK 999	UNP Q64096
C	1700	GLU	GLY	SEE REMARK 999	UNP Q64096
C	1701	LEU	VAL	SEE REMARK 999	UNP Q64096
C	1889	PHE	TYR	ENGINEERED	UNP Q64096
C	1968	GLU	-	CLONING ARTIFACT	UNP Q64096
C	1969	HIS	-	EXPRESSION TAG	UNP Q64096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1970	HIS	-	EXPRESSION TAG	UNP Q64096
C	1971	HIS	-	EXPRESSION TAG	UNP Q64096
C	1972	HIS	-	EXPRESSION TAG	UNP Q64096
C	1973	HIS	-	EXPRESSION TAG	UNP Q64096
C	1974	HIS	-	EXPRESSION TAG	UNP Q64096

- Molecule 2 is a protein called CDC42 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1471	943	239	282	7			
2	D	177	Total	C	N	O	S	0	0	0
			1379	888	220	264	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	SER	CYS	ENGINEERED	UNP P60953
D	1188	SER	CYS	ENGINEERED	UNP P60953

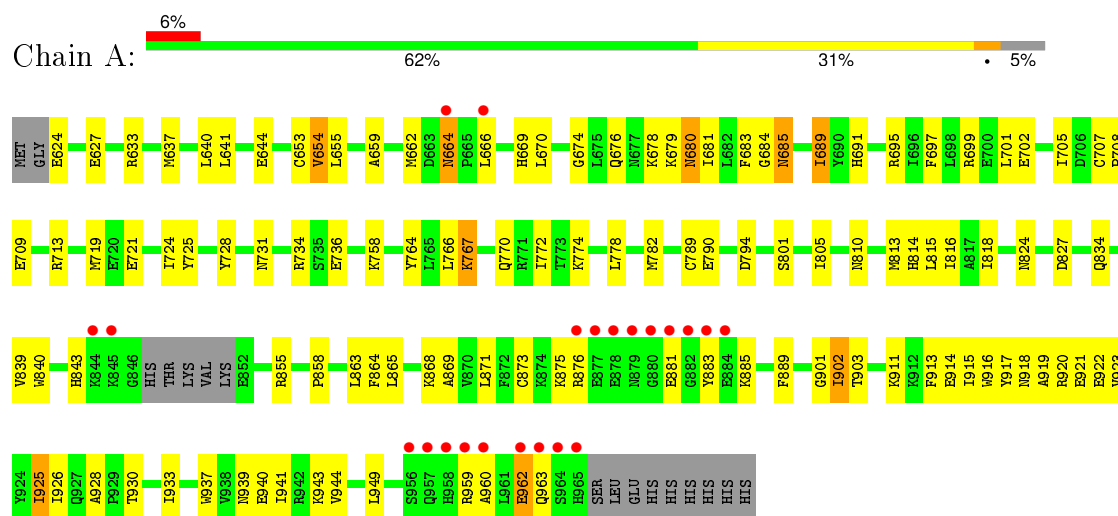
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	34	Total	O	0	0
			34	34		
3	C	24	Total	O	0	0
			24	24		
3	D	18	Total	O	0	0
			18	18		

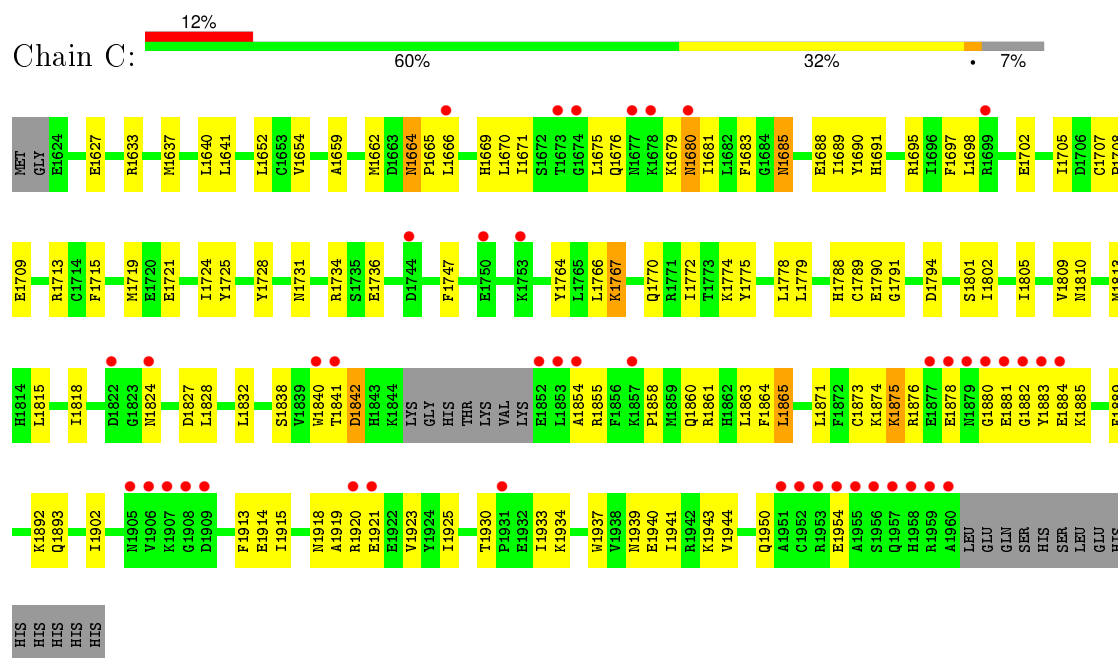
3 Residue-property plots

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

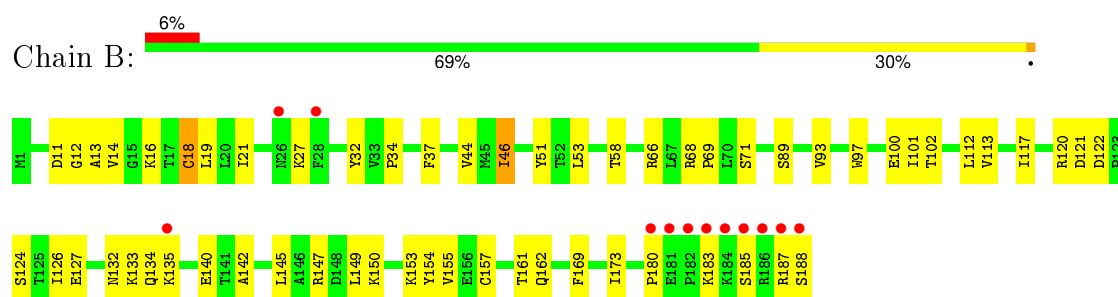
• Molecule 1: GUANINE NUCLEOTIDE EXCHANGE FACTOR DBS



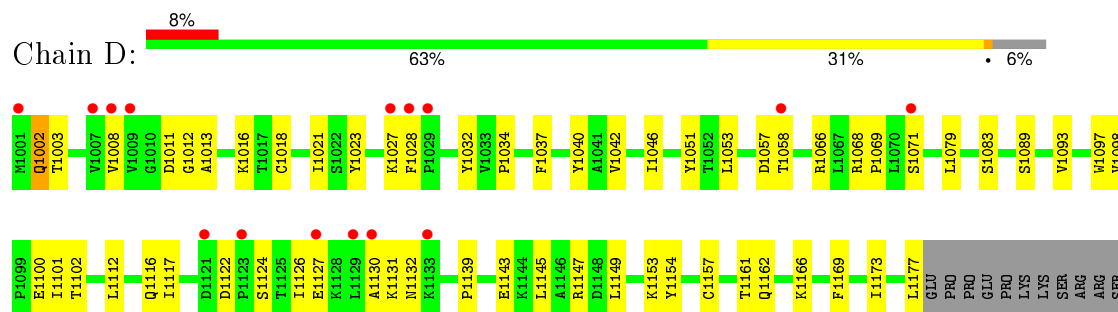
• Molecule 1: GUANINE NUCLEOTIDE EXCHANGE FACTOR DBS



• Molecule 2: CDC42 HOMOLOG



• Molecule 2: CDC42 HOMOLOG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.32Å 88.19Å 232.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 31.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.60) 99.7 (31.16-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.259 0.219 , 0.261	Depositor DCC
R_{free} test set	2165 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 43383 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2804	0.61	0/3767
1	C	0.36	0/2731	0.59	0/3672
2	B	0.42	0/1504	0.68	1/2044 (0.0%)
2	D	0.40	0/1409	0.66	0/1918
All	All	0.39	0/8448	0.63	1/11401 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	LEU	CA-CB-CG	5.33	127.55	115.30

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	2751	0	2733	118	0
1	C	2680	0	2655	101	0
2	B	1471	0	1494	49	0
2	D	1379	0	1396	42	0
3	A	39	0	0	2	0
3	B	34	0	0	2	0
3	C	24	0	0	4	0
3	D	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8396	0	8278	302	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 18.

All (302) 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:719:MET:HE2	1:A:801:SER:HB3	1.26	1.13
1:A:685:ASN:H	1:A:685:ASN:HD22	1.21	0.88
1:C:1685:ASN:HD22	1:C:1685:ASN:H	1.25	0.85
1:C:1664:ASN:HD21	1:C:1666:LEU:HG	1.43	0.83
1:C:1691:HIS:CG	1:C:1695:ARG:HH12	1.95	0.83
1:A:691:HIS:CG	1:A:695:ARG:HH12	1.99	0.81
1:A:685:ASN:O	1:A:689:ILE:HD13	1.81	0.81
1:A:815:LEU:O	1:A:818:ILE:HD13	1.82	0.80
1:A:664:ASN:HD21	1:A:666:LEU:HG	1.47	0.79
1:A:918:ASN:HB2	1:A:921:GLU:HG2	1.65	0.77
1:A:913:PHE:CE1	1:A:915:ILE:HD11	2.21	0.76
1:A:770:GLN:O	1:A:774:LYS:HG2	1.86	0.76
2:B:134:GLN:C	2:B:135:LYS:HD2	2.05	0.76
2:B:132:ASN:O	2:B:133:LYS:HG2	1.86	0.75
1:C:1881:GLU:HA	1:C:1885:LYS:HD3	1.67	0.75
1:C:1715:PHE:CD2	1:C:1802:ILE:HD11	2.22	0.74
1:C:1840:TRP:CE2	1:C:1858:PRO:HB3	2.22	0.74
1:C:1918:ASN:HB2	1:C:1921:GLU:HG2	1.69	0.73
1:A:758:LYS:HD3	3:B:2001:HOH:O	1.89	0.73
1:A:818:ILE:HD11	1:A:864:PHE:CZ	2.22	0.73
2:B:68:ARG:HB3	2:B:69:PRO:HD3	1.71	0.72
2:D:1068:ARG:HB3	2:D:1069:PRO:HD3	1.71	0.72
1:C:1709:GLU:HG2	1:C:1789:CYS:SG	2.30	0.71
2:B:18:CYS:HB2	3:B:2026:HOH:O	1.91	0.70
2:B:46:ILE:HD13	2:B:51:TYR:HB2	1.72	0.70
1:A:702:GLU:O	1:A:705:ILE:HG13	1.91	0.70
1:C:1779:LEU:HD12	1:C:1802:ILE:HD12	1.74	0.69
2:B:93:VAL:HG11	2:B:112:LEU:HD11	1.74	0.69
1:A:839:VAL:HG22	1:A:926:ILE:CD1	2.24	0.68
1:C:1876:ARG:HH22	1:C:1878:GLU:HB3	1.58	0.68
1:C:1920:ARG:NH1	1:C:1923:VAL:HG21	2.09	0.68
2:B:46:ILE:HD12	2:B:46:ILE:N	2.08	0.68
1:C:1702:GLU:O	1:C:1705:ILE:HG13	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:HIS:O	1:A:818:ILE:CD1	2.42	0.68
1:A:840:TRP:O	1:A:925:ILE:HD12	1.93	0.68
2:B:46:ILE:CD1	2:B:51:TYR:HB2	2.23	0.68
1:C:1689:ILE:HG12	1:C:1724:ILE:HD12	1.74	0.68
1:C:1770:GLN:O	1:C:1774:LYS:HG2	1.94	0.68
1:C:1719:MET:CE	1:C:1801:SER:HB3	2.24	0.67
1:A:902:ILE:HD13	1:A:903:THR:N	2.09	0.67
1:A:925:ILE:H	1:A:925:ILE:HD12	1.60	0.67
1:C:1764:TYR:HA	1:C:1767:LYS:HD3	1.77	0.67
2:D:1093:VAL:HG11	2:D:1112:LEU:HD11	1.77	0.66
1:A:719:MET:CE	1:A:801:SER:HB3	2.15	0.66
1:A:840:TRP:CB	1:A:925:ILE:HD13	2.25	0.66
1:A:840:TRP:HB3	1:A:925:ILE:HD13	1.78	0.65
1:A:689:ILE:HD12	1:A:724:ILE:HD12	1.76	0.65
1:A:685:ASN:HD21	1:A:728:TYR:HB2	1.60	0.65
1:A:633:ARG:NH2	3:A:2033:HOH:O	2.28	0.65
1:A:818:ILE:HD11	1:A:864:PHE:CE2	2.31	0.65
1:A:919:ALA:O	1:A:920:ARG:HB2	1.97	0.65
1:C:1919:ALA:O	1:C:1920:ARG:HB2	1.96	0.65
1:A:920:ARG:NH1	1:A:923:VAL:HG21	2.12	0.64
1:A:685:ASN:OD1	1:A:689:ILE:HD11	1.98	0.63
1:C:1876:ARG:NH2	1:C:1878:GLU:HB3	2.12	0.63
2:D:1042:VAL:HG23	2:D:1053:LEU:HB3	1.80	0.63
1:C:1719:MET:HE2	1:C:1801:SER:HB3	1.80	0.63
1:A:843:HIS:HD2	1:A:923:VAL:H	1.46	0.63
1:C:1721:GLU:O	1:C:1724:ILE:HG12	1.99	0.63
1:A:725:TYR:CB	1:A:772:ILE:HD12	2.29	0.62
1:A:815:LEU:C	1:A:818:ILE:HD13	2.20	0.62
1:A:840:TRP:HB2	1:A:925:ILE:HB	1.81	0.62
1:A:815:LEU:HA	1:A:818:ILE:HD13	1.82	0.61
1:A:680:ASN:HD22	1:A:680:ASN:N	1.96	0.61
2:B:122:ASP:O	2:B:126:ILE:HG12	1.99	0.61
1:A:937:TRP:O	1:A:941:ILE:HG12	2.01	0.61
2:B:169:PHE:O	2:B:173:ILE:HG12	2.00	0.61
1:A:764:TYR:HA	1:A:767:LYS:HD3	1.83	0.61
1:C:1937:TRP:O	1:C:1941:ILE:HG12	2.01	0.60
1:C:1680:ASN:HD22	1:C:1681:ILE:H	1.47	0.60
2:D:1101:ILE:HD12	2:D:1102:THR:N	2.17	0.60
1:C:1685:ASN:HD22	1:C:1685:ASN:N	1.93	0.59
2:D:1124:SER:O	2:D:1127:GLU:HB3	2.03	0.59
1:C:1881:GLU:CA	1:C:1885:LYS:HD3	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:HG23	2:B:46:ILE:HD11	1.83	0.59
1:A:902:ILE:HD13	1:A:903:THR:C	2.22	0.59
2:D:1161:THR:O	2:D:1162:GLN:HB2	2.02	0.59
2:D:1040:TYR:CE2	2:D:1042:VAL:HG13	2.38	0.59
1:A:915:ILE:HD13	1:A:926:ILE:HG12	1.84	0.58
1:C:1824:ASN:HB3	1:C:1827:ASP:OD2	2.03	0.58
1:C:1838:SER:HA	1:C:1860:GLN:NE2	2.19	0.58
1:A:925:ILE:N	1:A:925:ILE:HD12	2.18	0.58
2:B:53:LEU:HD22	2:B:173:ILE:HD11	1.84	0.58
2:B:147:ARG:HD3	2:B:188:SER:OXT	2.04	0.58
1:C:1685:ASN:HD21	1:C:1728:TYR:HB2	1.68	0.58
2:B:11:ASP:OD2	2:B:89:SER:HA	2.04	0.57
1:A:883:TYR:HB3	1:A:885:LYS:HE2	1.84	0.57
2:D:1046:ILE:HB	2:D:1051:TYR:CE1	2.40	0.56
1:C:1873:CYS:HB3	1:C:1889:PHE:HB3	1.86	0.56
1:A:875:LYS:HE3	3:A:2028:HOH:O	2.04	0.56
2:D:1021:ILE:HD13	2:D:1037:PHE:HD1	1.71	0.56
1:C:1633:ARG:NH2	3:C:2020:HOH:O	2.39	0.55
2:D:1011:ASP:OD2	2:D:1089:SER:HA	2.06	0.55
1:C:1680:ASN:HD22	1:C:1681:ILE:N	2.03	0.55
2:D:1131:LYS:HG2	2:D:1131:LYS:O	2.07	0.55
1:A:689:ILE:CD1	1:A:689:ILE:N	2.69	0.55
1:C:1875:LYS:HG2	1:C:1875:LYS:O	2.06	0.55
1:A:915:ILE:HD13	1:A:926:ILE:CG1	2.37	0.55
1:A:959:ARG:O	1:A:962:GLU:HB2	2.05	0.55
1:A:721:GLU:O	1:A:724:ILE:HG12	2.06	0.55
2:D:1018:CYS:SG	2:D:1028:PHE:HE1	2.30	0.55
1:A:915:ILE:HD12	1:A:915:ILE:N	2.22	0.55
2:B:46:ILE:HD13	2:B:51:TYR:CD1	2.41	0.55
1:C:1801:SER:O	1:C:1805:ILE:HD13	2.06	0.55
2:B:101:ILE:HD12	2:B:102:THR:N	2.22	0.55
1:A:633:ARG:HG2	1:A:782:MET:SD	2.47	0.54
1:C:1725:TYR:CG	1:C:1772:ILE:HD12	2.42	0.54
1:C:1939:ASN:O	1:C:1943:LYS:HG3	2.06	0.54
1:A:815:LEU:CA	1:A:818:ILE:HD13	2.37	0.54
1:A:719:MET:CE	1:A:805:ILE:HD13	2.38	0.54
1:A:689:ILE:CD1	1:A:724:ILE:HD12	2.38	0.54
1:A:818:ILE:N	1:A:818:ILE:HD12	2.22	0.54
2:D:1153:LYS:HG2	2:D:1154:TYR:N	2.23	0.54
1:A:814:HIS:O	1:A:818:ILE:HD12	2.07	0.54
1:A:725:TYR:CG	1:A:772:ILE:HD12	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1012:GLY:O	2:D:1013:ALA:HB3	2.08	0.54
1:A:813:MET:HB2	2:B:66:ARG:HG3	1.89	0.54
1:C:1685:ASN:H	1:C:1685:ASN:ND2	2.01	0.54
1:A:709:GLU:HG2	1:A:789:CYS:SG	2.47	0.54
1:C:1913:PHE:HE1	1:C:1915:ILE:HD11	1.71	0.54
1:A:839:VAL:HG22	1:A:926:ILE:HD13	1.90	0.53
2:D:1130:ALA:C	2:D:1132:ASN:H	2.10	0.53
1:A:824:ASN:HB3	1:A:827:ASP:OD2	2.09	0.53
1:A:960:ALA:C	1:A:962:GLU:H	2.12	0.53
1:C:1680:ASN:HD22	1:C:1680:ASN:N	2.06	0.53
1:A:685:ASN:ND2	1:A:685:ASN:H	2.01	0.53
1:A:873:CYS:HB3	1:A:889:PHE:HB3	1.90	0.53
2:B:134:GLN:O	2:B:135:LYS:HD2	2.08	0.53
2:D:1046:ILE:HB	2:D:1051:TYR:HE1	1.74	0.53
1:C:1779:LEU:CD1	1:C:1802:ILE:HD12	2.39	0.53
2:B:46:ILE:CD1	2:B:46:ILE:N	2.73	0.52
1:C:1725:TYR:CB	1:C:1772:ILE:HD12	2.40	0.52
1:A:669:HIS:CE1	1:A:670:LEU:HG	2.44	0.52
1:C:1637:MET:HB2	1:C:1708:PRO:HB3	1.91	0.52
1:A:843:HIS:CD2	1:A:923:VAL:H	2.26	0.52
1:A:813:MET:HB2	2:B:66:ARG:CG	2.40	0.52
1:C:1840:TRP:CZ2	1:C:1858:PRO:HB3	2.45	0.52
2:B:53:LEU:HD13	2:B:173:ILE:CD1	2.39	0.52
1:C:1640:LEU:HD13	1:C:1778:LEU:HD13	1.92	0.52
1:C:1838:SER:HA	1:C:1860:GLN:HE22	1.76	0.51
1:A:939:ASN:O	1:A:943:LYS:HG3	2.11	0.51
1:C:1815:LEU:HD12	1:C:1818:ILE:HD12	1.91	0.51
1:C:1864:PHE:HB2	1:C:1871:LEU:HB2	1.93	0.51
2:B:153:LYS:HG2	2:B:154:TYR:N	2.26	0.51
1:A:839:VAL:HG22	1:A:926:ILE:HD12	1.93	0.51
1:C:1940:GLU:O	1:C:1944:VAL:HG23	2.11	0.51
1:C:1880:GLY:O	1:C:1882:GLY:N	2.43	0.50
1:C:1689:ILE:CG1	1:C:1724:ILE:HD12	2.39	0.50
2:B:161:THR:O	2:B:162:GLN:HB2	2.12	0.50
1:A:624:GLU:CG	1:A:627:GLU:HB2	2.42	0.49
1:A:680:ASN:ND2	1:A:680:ASN:N	2.60	0.49
2:B:21:ILE:HD13	2:B:37:PHE:HD1	1.77	0.49
1:A:834:GLN:HA	1:A:863:LEU:O	2.13	0.49
1:C:1930:THR:OG1	1:C:1933:ILE:HG12	2.13	0.49
2:B:12:GLY:O	2:B:13:ALA:HB3	2.13	0.49
2:D:1002:GLN:O	2:D:1003:THR:HB	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:O	2:B:126:ILE:HD11	2.13	0.49
1:A:731:ASN:HD22	1:A:734:ARG:CZ	2.26	0.49
1:C:1664:ASN:HD22	1:C:1665:PRO:N	2.11	0.48
1:C:1664:ASN:ND2	1:C:1666:LEU:H	2.11	0.48
1:A:815:LEU:HA	1:A:818:ILE:CD1	2.43	0.48
1:A:840:TRP:CE2	1:A:858:PRO:HB3	2.48	0.48
1:C:1950:GLN:O	1:C:1954:GLU:HG3	2.12	0.48
2:D:1008:VAL:HG22	2:D:1079:LEU:HD12	1.95	0.48
1:A:881:GLU:C	1:A:883:TYR:H	2.16	0.48
1:C:1731:ASN:HD22	1:C:1734:ARG:NH1	2.12	0.48
1:C:1664:ASN:C	1:C:1664:ASN:HD22	2.15	0.48
1:A:731:ASN:HD22	1:A:734:ARG:NH1	2.11	0.48
1:A:633:ARG:HD3	1:A:709:GLU:HG3	1.96	0.48
2:D:1145:LEU:HD11	2:D:1149:LEU:HD11	1.95	0.48
1:A:637:MET:HB2	1:A:708:PRO:HB3	1.96	0.47
2:B:16:LYS:HE3	2:B:58:THR:OG1	2.13	0.47
2:B:147:ARG:HB3	2:B:147:ARG:HH11	1.78	0.47
2:D:1117:ILE:HG12	2:D:1157:CYS:O	2.15	0.47
1:A:702:GLU:O	1:A:705:ILE:CG1	2.60	0.47
2:D:1145:LEU:HG	2:D:1149:LEU:HD12	1.97	0.47
1:A:713:ARG:HG2	1:A:794:ASP:OD2	2.14	0.47
1:C:1659:ALA:O	1:C:1679:LYS:HE2	2.15	0.47
1:C:1764:TYR:HA	1:C:1767:LYS:CD	2.44	0.47
1:C:1918:ASN:HB2	1:C:1921:GLU:CG	2.43	0.46
1:A:876:ARG:HB3	1:A:876:ARG:HE	1.58	0.46
1:A:689:ILE:H	1:A:689:ILE:CD1	2.29	0.46
1:C:1652:LEU:HB2	1:C:1690:TYR:CE1	2.51	0.46
1:A:685:ASN:N	1:A:685:ASN:HD22	1.94	0.46
2:B:46:ILE:HD13	2:B:51:TYR:CB	2.44	0.46
2:D:1068:ARG:HD2	2:D:1100:GLU:OE2	2.15	0.46
1:C:1832:LEU:HB2	1:C:1865:LEU:HD13	1.96	0.46
1:C:1810:ASN:OD1	2:D:1066:ARG:HB2	2.16	0.46
1:A:662:MET:O	1:A:676:GLN:HG3	2.15	0.45
1:C:1841:THR:O	1:C:1842:ASP:HB2	2.16	0.45
1:C:1671:ILE:HG13	1:C:1675:LEU:HD23	1.98	0.45
1:C:1788:HIS:HE1	3:C:2058:HOH:O	1.99	0.45
1:C:1654:VAL:HG13	1:C:1683:PHE:HE2	1.81	0.45
1:A:918:ASN:HB2	1:A:921:GLU:CG	2.42	0.45
1:A:699:ARG:HH11	1:A:699:ARG:HG3	1.82	0.45
1:C:1691:HIS:ND1	1:C:1695:ARG:NH1	2.57	0.45
2:B:46:ILE:HD13	2:B:51:TYR:CG	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1662:MET:O	1:C:1676:GLN:HG3	2.17	0.45
2:D:1122:ASP:O	2:D:1126:ILE:HG13	2.17	0.45
1:C:1920:ARG:HH12	1:C:1923:VAL:HG21	1.81	0.45
2:B:117:ILE:HG12	2:B:157:CYS:O	2.17	0.45
2:D:1169:PHE:O	2:D:1173:ILE:HG13	2.17	0.44
1:A:719:MET:HE3	1:A:805:ILE:HD13	1.98	0.44
1:A:940:GLU:O	1:A:944:VAL:HG23	2.17	0.44
1:A:654:VAL:HG13	1:A:683:PHE:HE2	1.82	0.44
1:C:1854:ALA:O	1:C:1855:ARG:CZ	2.66	0.44
2:D:1040:TYR:HE2	2:D:1042:VAL:CG1	2.29	0.44
2:D:1083:SER:OG	2:D:1116:GLN:NE2	2.51	0.44
2:D:1016:LYS:HE3	2:D:1058:THR:OG1	2.17	0.44
2:B:140:GLU:CD	2:B:140:GLU:H	2.21	0.44
1:C:1691:HIS:CG	1:C:1695:ARG:NH1	2.75	0.44
1:C:1680:ASN:ND2	1:C:1681:ILE:N	2.64	0.44
1:A:960:ALA:O	1:A:963:GLN:HG3	2.17	0.44
2:B:124:SER:O	2:B:127:GLU:HB3	2.18	0.44
1:A:689:ILE:HD12	1:A:689:ILE:N	2.33	0.44
2:D:1032:TYR:O	2:D:1034:PRO:HD3	2.18	0.44
1:C:1775:TYR:HB3	1:C:1802:ILE:HD13	2.00	0.43
2:D:1040:TYR:CE2	2:D:1042:VAL:CG1	3.00	0.43
1:C:1828:LEU:CD1	1:C:1871:LEU:HD11	2.48	0.43
2:D:1147:ARG:HB3	2:D:1147:ARG:HH11	1.83	0.43
1:A:813:MET:HE2	2:B:66:ARG:HB3	1.99	0.43
1:C:1664:ASN:ND2	1:C:1664:ASN:C	2.71	0.43
1:C:1691:HIS:CB	1:C:1695:ARG:NH1	2.82	0.43
1:C:1863:LEU:HA	1:C:1871:LEU:O	2.18	0.43
1:C:1633:ARG:HD3	1:C:1709:GLU:HG3	2.01	0.43
2:D:1130:ALA:C	2:D:1132:ASN:N	2.71	0.43
1:C:1713:ARG:HG2	1:C:1794:ASP:OD2	2.18	0.43
1:A:674:GLY:O	1:A:678:LYS:HG3	2.19	0.43
1:C:1861:ARG:HG2	1:C:1861:ARG:HH11	1.83	0.43
1:C:1698:LEU:O	1:C:1702:GLU:HG3	2.18	0.43
1:C:1669:HIS:CE1	1:C:1670:LEU:HG	2.53	0.43
1:A:818:ILE:N	1:A:818:ILE:CD1	2.82	0.43
1:A:915:ILE:CD1	1:A:926:ILE:HG12	2.49	0.43
1:A:840:TRP:O	1:A:925:ILE:CD1	2.64	0.43
1:A:911:LYS:HD2	1:A:928:ALA:O	2.19	0.43
1:C:1791:GLY:HA2	3:C:2050:HOH:O	2.19	0.43
1:C:1914:GLU:OE1	1:C:1920:ARG:NH2	2.52	0.42
1:A:680:ASN:HD22	1:A:681:ILE:H	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1809:VAL:O	1:C:1813:MET:HG2	2.18	0.42
1:A:816:ILE:C	1:A:816:ILE:HD12	2.40	0.42
1:C:1766:LEU:HD11	2:D:1071:SER:HA	2.01	0.42
2:D:1068:ARG:HD3	2:D:1097:TRP:HZ3	1.84	0.42
1:A:764:TYR:HA	1:A:767:LYS:CD	2.46	0.42
2:D:1023:TYR:HE1	2:D:1166:LYS:HD3	1.84	0.42
1:C:1680:ASN:ND2	1:C:1680:ASN:N	2.66	0.42
2:D:1139:PRO:O	2:D:1143:GLU:HG3	2.18	0.42
1:C:1662:MET:HG2	1:C:1747:PHE:CE2	2.54	0.42
1:C:1731:ASN:ND2	1:C:1734:ARG:HD2	2.34	0.42
1:A:949:LEU:HD11	1:C:1627:GLU:OE1	2.19	0.42
2:B:68:ARG:HD3	2:B:97:TRP:HZ3	1.84	0.42
1:A:624:GLU:HG3	1:A:627:GLU:H	1.85	0.42
1:A:640:LEU:HD13	1:A:778:LEU:HD13	2.00	0.42
1:C:1838:SER:CB	1:C:1860:GLN:HE22	2.32	0.42
2:D:1153:LYS:CG	2:D:1154:TYR:N	2.82	0.42
2:B:149:LEU:O	2:B:150:LYS:HB2	2.20	0.42
1:A:902:ILE:HG12	1:A:914:GLU:O	2.19	0.42
1:A:683:PHE:O	1:A:684:GLY:C	2.57	0.42
2:B:101:ILE:HD12	2:B:101:ILE:C	2.40	0.41
1:A:655:LEU:O	1:A:659:ALA:HB3	2.20	0.41
1:A:962:GLU:OE1	1:A:962:GLU:HA	2.20	0.41
2:B:145:LEU:HD11	2:B:149:LEU:HD11	2.02	0.41
2:B:150:LYS:HE2	2:B:185:SER:OG	2.20	0.41
1:C:1685:ASN:ND2	1:C:1685:ASN:N	2.64	0.41
1:C:1688:GLU:O	1:C:1691:HIS:HB2	2.20	0.41
1:C:1731:ASN:HD22	1:C:1734:ARG:CZ	2.33	0.41
1:C:1691:HIS:HB3	1:C:1695:ARG:NH1	2.35	0.41
1:A:664:ASN:C	1:A:664:ASN:HD22	2.23	0.41
2:D:1098:VAL:HG21	2:D:1149:LEU:HD13	2.02	0.41
1:A:868:LYS:O	1:A:869:ALA:HB2	2.20	0.41
1:C:1633:ARG:NH1	3:C:2040:HOH:O	2.53	0.41
1:A:731:ASN:ND2	1:A:734:ARG:HD2	2.36	0.41
2:B:113:VAL:HA	2:B:155:VAL:O	2.20	0.41
1:A:644:GLU:HG2	1:A:701:LEU:HD12	2.01	0.41
1:C:1840:TRP:HB2	1:C:1925:ILE:HB	2.02	0.41
2:B:153:LYS:CG	2:B:154:TYR:N	2.84	0.41
2:B:135:LYS:N	2:B:135:LYS:HD2	2.34	0.41
2:B:68:ARG:HD2	2:B:100:GLU:OE2	2.20	0.41
2:D:1101:ILE:HD12	2:D:1101:ILE:C	2.41	0.41
1:C:1902:ILE:HG13	1:C:1914:GLU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ASP:O	2:B:14:VAL:HG22	2.20	0.41
1:A:901:GLY:HA3	1:A:916:TRP:CZ3	2.56	0.41
1:A:766:LEU:HD11	2:B:71:SER:HA	2.03	0.41
1:C:1874:LYS:HB2	1:C:1892:LYS:HD3	2.02	0.41
1:A:915:ILE:CD1	1:A:926:ILE:CG1	2.99	0.40
1:C:1878:GLU:O	1:C:1878:GLU:HG3	2.21	0.40
1:C:1913:PHE:CD2	1:C:1934:LYS:HG2	2.56	0.40
1:A:659:ALA:O	1:A:679:LYS:HE2	2.22	0.40
2:D:1040:TYR:CD2	2:D:1042:VAL:HG13	2.56	0.40
1:A:863:LEU:HA	1:A:871:LEU:O	2.21	0.40
1:A:917:TYR:HB3	1:A:922:GLU:HB2	2.03	0.40
1:C:1691:HIS:CB	1:C:1695:ARG:HH12	2.34	0.40
2:B:46:ILE:HD11	2:B:51:TYR:HB2	1.99	0.40
1:A:725:TYR:HB2	1:A:772:ILE:HD12	2.03	0.40
2:D:1018:CYS:SG	2:D:1028:PHE:CE1	3.12	0.40
1:A:810:ASN:OD1	2:B:66:ARG:HB2	2.20	0.40
2:B:142:ALA:HB1	2:B:154:TYR:CE1	2.57	0.40
2:B:32:TYR:O	2:B:34:PRO:HD3	2.21	0.40
1:A:691:HIS:HB3	1:A:695:ARG:NH1	2.35	0.40
1:C:1705:ILE:H	1:C:1705:ILE:HG13	1.60	0.40
1:A:633:ARG:CD	1:A:709:GLU:HG3	2.51	0.40
2:D:1057:ASP:OD1	2:D:1058:THR:N	2.54	0.40
1:A:930:THR:OG1	1:A:933:ILE:HG12	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	333/353 (94%)	317 (95%)	16 (5%)	0	100	100
1	C	326/353 (92%)	308 (94%)	15 (5%)	3 (1%)	21	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	186/188 (99%)	171 (92%)	12 (6%)	3 (2%)	12	24
2	D	175/188 (93%)	158 (90%)	17 (10%)	0	100	100
All	All	1020/1082 (94%)	954 (94%)	60 (6%)	6 (1%)	30	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	180	PRO
1	C	1842	ASP
1	C	1884	GLU
1	C	1875	LYS
2	B	183	LYS
2	B	187	ARG

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	301/316 (95%)	284 (94%)	17 (6%)	26	50
1	C	291/316 (92%)	279 (96%)	12 (4%)	37	66
2	B	168/168 (100%)	164 (98%)	4 (2%)	57	82
2	D	157/168 (94%)	154 (98%)	3 (2%)	65	86
All	All	917/968 (95%)	881 (96%)	36 (4%)	39	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	641	LEU
1	A	653	CYS
1	A	654	VAL
1	A	664	ASN
1	A	680	ASN
1	A	685	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	689	ILE
1	A	697	PHE
1	A	707	CYS
1	A	736	GLU
1	A	767	LYS
1	A	790	GLU
1	A	855	ARG
1	A	865	LEU
1	A	902	ILE
1	A	925	ILE
1	A	962	GLU
2	B	18	CYS
2	B	27	LYS
2	B	46	ILE
2	B	121	ASP
1	C	1641	LEU
1	C	1664	ASN
1	C	1680	ASN
1	C	1685	ASN
1	C	1697	PHE
1	C	1707	CYS
1	C	1736	GLU
1	C	1767	LYS
1	C	1790	GLU
1	C	1865	LEU
1	C	1883	TYR
1	C	1893	GLN
2	D	1002	GLN
2	D	1027	LYS
2	D	1177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	664	ASN
1	A	677	ASN
1	A	680	ASN
1	A	685	ASN
1	A	731	ASN
1	A	843	HIS
1	A	893	GLN
1	A	948	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	116	GLN
2	B	134	GLN
1	C	1664	ASN
1	C	1677	ASN
1	C	1680	ASN
1	C	1685	ASN
1	C	1731	ASN
1	C	1860	GLN
1	C	1893	GLN
1	C	1948	GLN
2	D	1104	HIS
2	D	1116	GLN
2	D	1134	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	337/353 (95%)	0.18	22 (6%) 22 16	28, 51, 102, 143	0
1	C	330/353 (93%)	0.60	44 (13%) 4 3	31, 58, 114, 138	0
2	B	188/188 (100%)	0.22	12 (6%) 23 17	29, 44, 90, 140	0
2	D	177/188 (94%)	0.30	15 (8%) 13 9	33, 50, 93, 106	0
All	All	1032/1082 (95%)	0.34	93 (9%) 12 8	28, 52, 101, 143	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	182	PRO	9.0
1	C	1853	LEU	8.7
1	A	880	GLY	7.8
1	C	1908	GLY	7.7
1	C	1854	ALA	7.6
2	B	188	SER	7.4
1	C	1883	TYR	7.2
1	A	881	GLU	7.2
2	D	1001	MET	7.2
1	C	1852	GLU	7.0
1	C	1880	GLY	6.5
1	A	963	GLN	6.4
1	C	1882	GLY	6.3
1	A	882	GLY	6.1
2	B	181	GLU	5.9
1	A	883	TYR	5.9
1	C	1958	HIS	5.8
1	C	1953	ARG	5.6
2	B	186	ARG	5.6
1	C	1879	ASN	5.6
1	A	879	ASN	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1878	GLU	5.5
2	B	180	PRO	5.4
1	A	878	GLU	5.4
1	A	960	ALA	5.1
1	A	965	HIS	5.1
1	C	1881	GLU	5.1
1	A	877	GLU	4.6
1	C	1877	GLU	4.6
1	C	1909	ASP	4.6
2	D	1133	LYS	4.5
1	A	964	SER	4.5
1	C	1956	SER	4.4
2	B	184	LYS	4.4
1	A	845	LYS	4.3
1	C	1955	ALA	4.3
1	C	1907	LYS	4.1
1	C	1954	GLU	4.1
1	C	1921	GLU	3.8
1	C	1673	THR	3.8
1	C	1905	ASN	3.8
1	C	1906	VAL	3.6
1	C	1822	ASP	3.6
1	A	884	GLU	3.6
1	C	1959	ARG	3.6
1	C	1666	LEU	3.5
1	C	1952	CYS	3.4
1	C	1957	GLN	3.3
1	C	1753	LYS	3.2
1	C	1960	ALA	3.2
2	D	1127	GLU	3.1
2	B	183	LYS	3.1
2	B	187	ARG	3.0
1	A	844	LYS	3.0
2	D	1008	VAL	3.0
2	B	185	SER	2.8
1	A	958	HIS	2.8
1	C	1824	ASN	2.7
1	C	1951	ALA	2.7
2	D	1121	ASP	2.7
1	C	1884	GLU	2.6
1	C	1699	ARG	2.6
1	A	962	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	135	LYS	2.6
1	C	1931	PRO	2.5
1	C	1677	ASN	2.5
1	A	664	ASN	2.4
1	A	666	LEU	2.4
1	A	876	ARG	2.4
2	D	1123	PRO	2.4
2	D	1058	THR	2.4
1	A	956	SER	2.3
1	A	959	ARG	2.3
2	D	1129	LEU	2.3
1	C	1744	ASP	2.3
2	D	1027	LYS	2.3
1	C	1674	GLY	2.2
1	C	1840	TRP	2.2
1	A	957	GLN	2.2
2	B	26	ASN	2.1
2	D	1071	SER	2.1
1	C	1920	ARG	2.1
1	C	1680	ASN	2.1
2	D	1009	VAL	2.1
2	D	1029	PRO	2.1
1	C	1678	LYS	2.1
2	D	1007	VAL	2.0
2	D	1028	PHE	2.0
1	C	1841	THR	2.0
1	C	1857	LYS	2.0
2	D	1130	ALA	2.0
1	C	1750	GLU	2.0
2	B	28	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.