Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:35 PM GMT

PDB ID	:	1KZ7
Title	:	Crystal Structure of the DH/PH Fragment of Murine Dbs in Complex with the Placental Isoform of Human Cdc42
Authors	:	Rossman, K.L.; Worthylake, D.K.; Snyder, J.T.; Siderovski, D.P.; Campbell, S.L.; Sondek, J.
Deposited on	:	2002-02-06
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

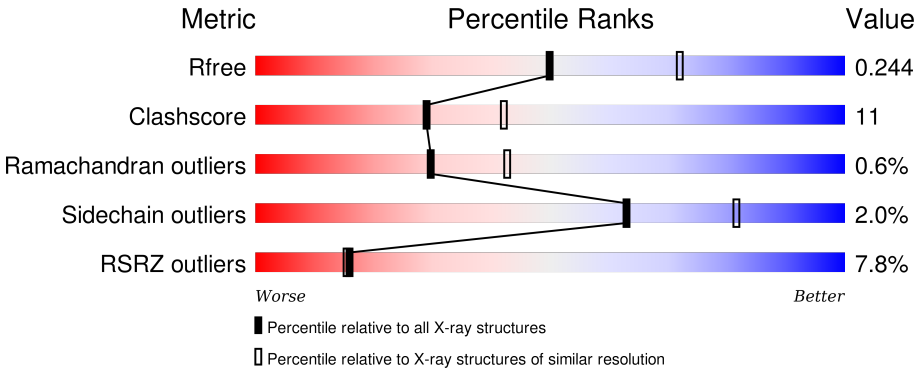
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	353	7% 69% 24% • 5%
1	C	353	8% 67% 26% • 7%
2	B	188	3% 83% 17%
2	D	188	12% 72% 22% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8598 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	Se	0	0	0
			2748	1741	474	512	11	10			
1	C	330	Total	C	N	O	S	Se	0	0	0
			2677	1700	457	499	11	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	MSE	-	SEE REMARK 999	UNP Q64096
A	637	MSE	MET	modified residue	UNP Q64096
A	662	MSE	MET	modified residue	UNP Q64096
A	667	MSE	MET	modified residue	UNP Q64096
A	686	MSE	MET	modified residue	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	719	MSE	MET	modified residue	UNP Q64096
A	782	MSE	MET	modified residue	UNP Q64096
A	813	MSE	MET	modified residue	UNP Q64096
A	833	MSE	MET	modified residue	UNP Q64096
A	859	MSE	MET	modified residue	UNP Q64096
A	897	MSE	MET	modified residue	UNP Q64096
A	940	ALA	GLU	SEE REMARK 999	UNP Q64096
A	968	GLU	-	EXPRESSION TAG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1622	MSE	-	SEE REMARK 999	UNP Q64096
C	1637	MSE	MET	modified residue	UNP Q64096
C	1662	MSE	MET	modified residue	UNP Q64096
C	1667	MSE	MET	modified residue	UNP Q64096
C	1686	MSE	MET	modified residue	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	1719	MSE	MET	modified residue	UNP Q64096
C	1782	MSE	MET	modified residue	UNP Q64096
C	1813	MSE	MET	modified residue	UNP Q64096
C	1833	MSE	MET	modified residue	UNP Q64096
C	1859	MSE	MET	modified residue	UNP Q64096
C	1897	MSE	MET	modified residue	UNP Q64096
C	1940	ALA	GLU	SEE REMARK 999	UNP Q64096
C	1968	GLU	-	EXPRESSION TAG	UNP Q64096
C	1969	HIS	-	EXPRESSION TAG	UNP Q64096
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.

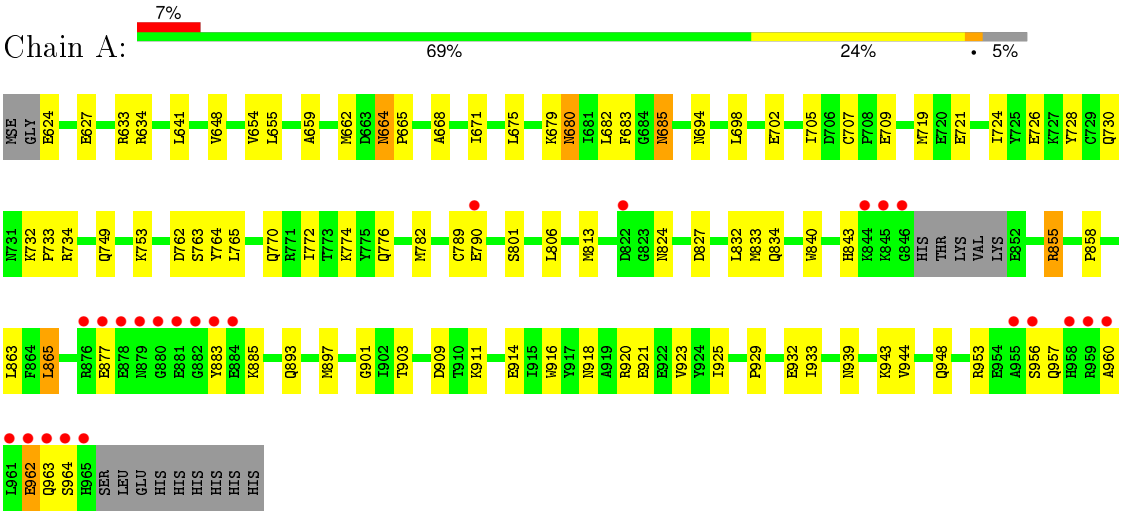
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	97	Total O 97 97	0	0
3	C	87	Total O 87 87	0	0
3	D	47	Total O 47 47	0	0

3 Residue-property plots (i)

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.

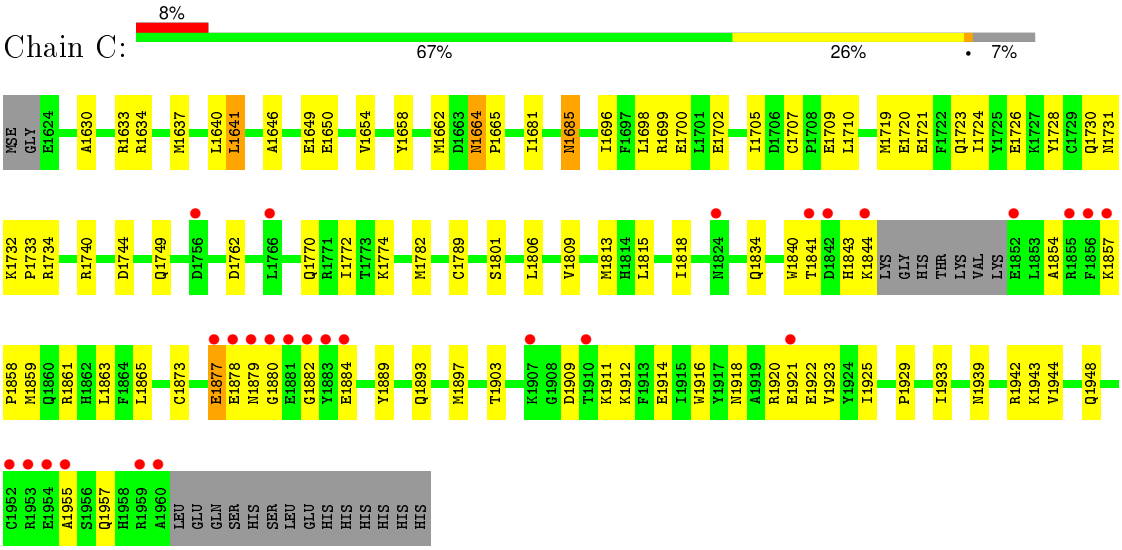
- Molecule 1: GUANINE NUCLEOTIDE EXCHANGE FACTOR DBS

Chain A:



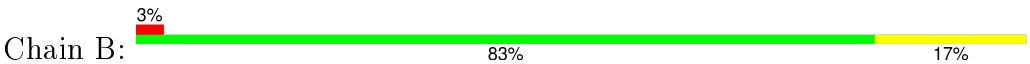
- Molecule 1: GUANINE NUCLEOTIDE EXCHANGE FACTOR DBS

Chain C:

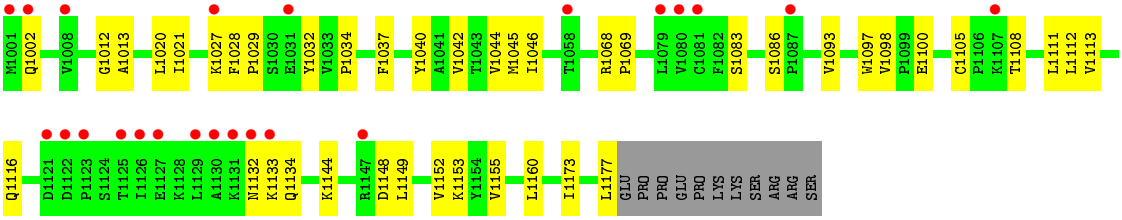


- Molecule 2: CDC42 HOMOLOG

Chain B:



- Molecule 2: CDC42 HOMOLOG



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.50Å 87.98Å 230.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 29.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.99-2.40) 91.3 (29.51-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.239 0.203 , 0.244	Depositor DCC
R_{free} test set	2460 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49134 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8598	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 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	0.34	0/2791	0.58	0/3734
1	C	0.35	0/2718	0.56	0/3639
2	B	0.37	0/1504	0.65	0/2044
2	D	0.32	0/1409	0.61	0/1918
All	All	0.34	0/8422	0.59	0/11335

There are no bond length outliers.

There are no bond angle outliers.

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	2748	0	2732	68	0
1	C	2677	0	2654	72	0
2	B	1471	0	1494	23	0
2	D	1379	0	1396	28	0
3	A	92	0	0	6	0
3	B	97	0	0	3	0
3	C	87	0	0	5	0
3	D	47	0	0	0	0
All	All	8598	0	8276	189	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 11.

All (189) 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:1719:MSE:HE2	1:C:1801:SER:HB3	1.41	1.03
1:A:929:PRO:HG2	1:A:933:ILE:HD12	1.55	0.88
1:C:1731:ASN:HD22	1:C:1734:ARG:HH21	1.24	0.85
1:A:685:ASN:H	1:A:685:ASN:HD22	1.24	0.84
1:A:707:CYS:HB3	3:A:2271:HOH:O	1.78	0.82
1:C:1903:THR:HB	1:C:1914:GLU:HB2	1.61	0.82
2:B:147:ARG:HB3	2:B:147:ARG:HH11	1.45	0.79
1:C:1939:ASN:O	1:C:1943:LYS:HG2	1.83	0.78
1:C:1685:ASN:H	1:C:1685:ASN:HD22	1.31	0.78
1:A:633:ARG:HD3	1:A:709:GLU:HG3	1.65	0.77
1:A:719:MSE:HE2	1:A:801:SER:HB3	1.68	0.76
1:A:897:MSE:HE2	1:A:944:VAL:HG12	1.70	0.73
1:C:1770:GLN:O	1:C:1774:LYS:HG2	1.89	0.73
2:D:1152:VAL:HG12	2:D:1153:LYS:HG3	1.71	0.72
1:A:897:MSE:HE2	1:A:944:VAL:CG1	2.20	0.72
2:D:1068:ARG:HB3	2:D:1069:PRO:HD3	1.73	0.69
1:A:939:ASN:O	1:A:943:LYS:HG2	1.91	0.69
1:C:1664:ASN:HD22	1:C:1665:PRO:N	1.91	0.69
2:B:120:ARG:O	2:B:126:ILE:HD11	1.93	0.69
2:D:1173:ILE:O	2:D:1177:LEU:HD13	1.91	0.69
1:C:1929:PRO:HG2	1:C:1933:ILE:HD12	1.75	0.69
1:C:1633:ARG:HG2	1:C:1782:MSE:SE	2.44	0.68
1:C:1841:THR:HB	1:C:1843:HIS:CE1	2.29	0.67
2:B:132:ASN:O	2:B:133:LYS:HG2	1.94	0.67
1:C:1897:MSE:HE2	1:C:1944:VAL:CG1	2.25	0.67
1:C:1762:ASP:HB3	3:C:2319:HOH:O	1.95	0.67
1:C:1749:GLN:HG3	3:C:2031:HOH:O	1.95	0.67
1:A:734:ARG:HD3	3:A:2224:HOH:O	1.95	0.67
1:A:633:ARG:HG2	1:A:782:MSE:SE	2.46	0.65
1:A:885:LYS:HG3	2:B:104:HIS:HA	1.79	0.65
1:C:1702:GLU:O	1:C:1705:ILE:HG13	1.97	0.65
1:C:1719:MSE:CE	1:C:1801:SER:HB3	2.24	0.65
1:A:770:GLN:O	1:A:774:LYS:HG2	1.97	0.65
1:A:664:ASN:HD22	1:A:665:PRO:HD2	1.63	0.64
1:C:1698:LEU:O	1:C:1702:GLU:HG3	1.97	0.64
2:B:68:ARG:HB3	2:B:69:PRO:HD3	1.79	0.64
1:C:1878:GLU:O	1:C:1878:GLU:HG3	1.98	0.64
1:A:953:ARG:O	1:A:957:GLN:HG3	1.98	0.64
1:C:1772:ILE:HG13	1:C:1806:LEU:HD21	1.80	0.62
2:D:1068:ARG:HD2	2:D:1100:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LYS:HB3	3:B:2305:HOH:O	1.99	0.62
1:C:1664:ASN:HD22	1:C:1665:PRO:CD	2.12	0.62
1:A:918:ASN:HB2	1:A:921:GLU:HG2	1.82	0.62
1:A:671:ILE:HG13	1:A:675:LEU:HD23	1.82	0.61
1:A:925:ILE:N	1:A:925:ILE:HD12	2.15	0.61
1:C:1897:MSE:HE2	1:C:1944:VAL:HG11	1.82	0.61
1:A:763:SER:HB3	3:A:2302:HOH:O	1.99	0.61
1:C:1646:ALA:O	1:C:1650:GLU:HG3	2.01	0.60
1:C:1918:ASN:HB2	1:C:1921:GLU:HG2	1.82	0.60
1:C:1740:ARG:HD3	1:C:1882:GLY:HA2	1.84	0.60
2:D:1083:SER:HB3	2:D:1086:SER:HB3	1.83	0.60
1:C:1685:ASN:HD21	1:C:1728:TYR:HB2	1.66	0.60
1:C:1731:ASN:HD22	1:C:1734:ARG:NH2	1.96	0.60
1:C:1633:ARG:HD3	1:C:1709:GLU:HG3	1.83	0.60
1:C:1720:GLU:O	1:C:1723:GLN:HG2	2.03	0.58
1:A:855:ARG:HB2	1:A:855:ARG:HH11	1.68	0.58
1:A:909:ASP:OD1	1:A:911:LYS:HG2	2.04	0.58
1:A:633:ARG:NH2	3:A:2256:HOH:O	2.27	0.58
2:D:1027:LYS:C	2:D:1027:LYS:HD2	2.23	0.58
2:D:1111:LEU:HD23	2:D:1152:VAL:HB	1.86	0.58
1:C:1859:MSE:HE3	1:C:1861:ARG:HG3	1.85	0.58
1:C:1731:ASN:ND2	1:C:1734:ARG:HE	2.02	0.57
1:C:1685:ASN:HD22	1:C:1685:ASN:N	1.97	0.57
1:A:824:ASN:HB3	1:A:827:ASP:OD2	2.05	0.57
1:C:1726:GLU:O	1:C:1730:GLN:HG3	2.05	0.56
1:C:1841:THR:HB	1:C:1843:HIS:ND1	2.19	0.56
1:A:698:LEU:O	1:A:702:GLU:HG3	2.04	0.56
1:C:1920:ARG:NH1	1:C:1923:VAL:HG21	2.20	0.56
1:C:1840:TRP:CE2	1:C:1858:PRO:HB3	2.41	0.56
1:C:1637:MSE:HE2	1:C:1641:LEU:HD13	1.89	0.55
1:A:664:ASN:HD22	1:A:665:PRO:CD	2.20	0.55
2:D:1098:VAL:HG21	2:D:1149:LEU:HD13	1.88	0.55
1:C:1699:ARG:HG2	3:C:2264:HOH:O	2.07	0.55
1:A:641:LEU:HD11	1:A:702:GLU:HG2	1.87	0.55
1:A:762:ASP:HA	1:A:765:LEU:HD12	1.90	0.54
1:A:772:ILE:HG13	1:A:806:LEU:HD21	1.90	0.54
2:D:1093:VAL:HG11	2:D:1112:LEU:HD11	1.90	0.54
2:B:12:GLY:O	2:B:13:ALA:HB3	2.07	0.54
1:A:721:GLU:O	1:A:724:ILE:HG12	2.08	0.53
1:A:685:ASN:HD21	1:A:728:TYR:HB2	1.72	0.53
2:B:40:TYR:HE2	2:B:42:VAL:HG22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:TYR:CE2	2:B:42:VAL:HG22	2.44	0.53
1:A:843:HIS:HD2	1:A:923:VAL:H	1.57	0.53
1:C:1909:ASP:HB3	1:C:1912:LYS:HG3	1.91	0.53
1:A:685:ASN:N	1:A:685:ASN:HD22	1.95	0.52
2:B:180:PRO:HA	3:B:2305:HOH:O	2.09	0.52
1:A:680:ASN:HD22	1:A:680:ASN:H	1.55	0.52
1:C:1925:ILE:HD12	1:C:1925:ILE:N	2.23	0.52
1:A:634:ARG:NH2	1:A:705:ILE:O	2.38	0.52
2:B:133:LYS:HG3	2:B:133:LYS:O	2.10	0.52
1:C:1696:ILE:O	1:C:1700:GLU:HG3	2.10	0.52
1:A:962:GLU:C	1:A:964:SER:H	2.13	0.52
1:C:1685:ASN:H	1:C:1685:ASN:ND2	2.05	0.51
1:A:707:CYS:SG	1:A:709:GLU:OE1	2.68	0.51
1:C:1664:ASN:HD22	1:C:1665:PRO:HD2	1.75	0.51
1:A:702:GLU:O	1:A:705:ILE:HG13	2.11	0.51
1:C:1840:TRP:HA	1:C:1854:ALA:HB3	1.93	0.51
2:D:1068:ARG:HD3	2:D:1097:TRP:HZ3	1.76	0.51
2:D:1012:GLY:O	2:D:1013:ALA:HB3	2.12	0.50
1:A:901:GLY:HA3	1:A:916:TRP:CZ3	2.46	0.50
1:C:1857:LYS:HD2	1:C:1858:PRO:HD2	1.92	0.50
1:C:1633:ARG:NH2	3:C:2257:HOH:O	2.32	0.50
1:A:749:GLN:O	1:A:753:LYS:HG3	2.12	0.50
1:A:901:GLY:HA3	1:A:916:TRP:CH2	2.47	0.50
1:A:840:TRP:CE2	1:A:858:PRO:HB3	2.46	0.50
1:A:726:GLU:O	1:A:730:GLN:HG3	2.10	0.50
1:C:1843:HIS:CD2	1:C:1922:GLU:HG2	2.46	0.50
1:C:1664:ASN:C	1:C:1664:ASN:HD22	2.15	0.49
1:A:877:GLU:O	1:A:877:GLU:HG2	2.11	0.49
1:A:624:GLU:HG3	1:A:627:GLU:H	1.76	0.49
1:A:682:LEU:HD23	1:A:683:PHE:CE1	2.47	0.48
1:C:1649:GLU:HG3	3:C:2134:HOH:O	2.13	0.48
1:C:1699:ARG:HG3	1:C:1699:ARG:HH11	1.79	0.48
1:C:1942:ARG:HH11	1:C:1942:ARG:HG2	1.78	0.48
1:C:1815:LEU:HD12	1:C:1818:ILE:HD12	1.96	0.48
2:D:1105:CYS:HB3	2:D:1108:THR:OG1	2.13	0.48
2:B:152:VAL:O	2:B:153:LYS:HG3	2.13	0.48
2:D:1020:LEU:HD13	2:D:1037:PHE:CD2	2.49	0.48
1:A:685:ASN:ND2	1:A:685:ASN:H	2.03	0.47
1:C:1732:LYS:N	1:C:1733:PRO:HD2	2.29	0.47
2:B:68:ARG:CD	2:B:100:GLU:OE2	2.62	0.47
1:A:920:ARG:NH1	1:A:923:VAL:HG21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:SER:O	1:A:960:ALA:HB2	2.13	0.47
2:D:1045:MET:C	2:D:1046:ILE:HD12	2.35	0.47
1:A:671:ILE:HD11	1:A:675:LEU:HG	1.96	0.47
1:A:662:MSE:HE2	1:A:675:LEU:HG	1.97	0.47
1:A:843:HIS:CD2	1:A:923:VAL:H	2.32	0.47
1:A:789:CYS:HB3	3:A:2260:HOH:O	2.14	0.47
2:B:130:ALA:C	2:B:132:ASN:H	2.19	0.46
1:C:1929:PRO:HG2	1:C:1933:ILE:CD1	2.44	0.46
2:B:68:ARG:HD2	2:B:100:GLU:OE2	2.15	0.46
2:D:1021:ILE:CD1	2:D:1034:PRO:HB2	2.46	0.46
1:C:1840:TRP:CZ2	1:C:1858:PRO:HB3	2.51	0.46
2:B:187:ARG:O	2:B:188:SER:HB2	2.16	0.45
2:B:98:VAL:HB	2:B:99:PRO:HD3	1.98	0.45
2:D:1132:ASN:HB2	2:D:1134:GLN:HE21	1.82	0.45
1:A:834:GLN:HA	1:A:863:LEU:O	2.17	0.45
1:A:903:THR:HB	1:A:914:GLU:HB2	1.98	0.45
1:A:655:LEU:O	1:A:659:ALA:HB3	2.17	0.45
1:C:1658:TYR:O	1:C:1662:MSE:HG3	2.16	0.45
2:D:1144:LYS:HG2	2:D:1148:ASP:OD2	2.17	0.45
1:A:648:VAL:HG11	1:A:694:ASN:HD22	1.81	0.45
2:B:84:VAL:HG21	2:B:117:ILE:HA	1.99	0.44
1:C:1630:ALA:O	1:C:1634:ARG:HG3	2.17	0.44
2:D:1002:GLN:O	2:D:1002:GLN:HG3	2.18	0.44
2:D:1027:LYS:O	2:D:1027:LYS:HD2	2.18	0.44
1:C:1877:GLU:CD	1:C:1879:ASN:HD21	2.21	0.44
1:A:932:GLU:H	1:A:932:GLU:CD	2.20	0.44
1:C:1880:GLY:C	1:C:1882:GLY:H	2.20	0.43
2:B:166:LYS:HE3	3:B:2322:HOH:O	2.17	0.43
2:D:1068:ARG:NH1	2:D:1100:GLU:OE1	2.51	0.43
1:C:1709:GLU:HG2	1:C:1789:CYS:SG	2.59	0.43
1:C:1721:GLU:O	1:C:1724:ILE:HG12	2.19	0.43
2:D:1133:LYS:N	2:D:1133:LYS:HD3	2.33	0.43
1:C:1740:ARG:CD	1:C:1882:GLY:HA2	2.48	0.42
1:C:1955:ALA:C	1:C:1957:GLN:H	2.20	0.42
1:C:1809:VAL:O	1:C:1813:MSE:HG2	2.19	0.42
1:C:1844:LYS:O	1:C:1844:LYS:HG3	2.20	0.42
1:A:832:LEU:HB2	1:A:865:LEU:HD13	2.01	0.42
2:D:1083:SER:OG	2:D:1116:GLN:NE2	2.52	0.42
1:A:762:ASP:HB2	3:A:2240:HOH:O	2.18	0.42
1:C:1637:MSE:HE1	1:C:1640:LEU:HD23	2.00	0.42
1:A:813:MSE:HB2	2:B:66:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1029:PRO:HB3	2:D:1034:PRO:HD3	2.01	0.42
1:A:659:ALA:HB1	1:A:679:LYS:HE3	2.01	0.42
2:D:1040:TYR:CE2	2:D:1042:VAL:HG22	2.54	0.42
2:B:182:PRO:O	2:B:183:LYS:C	2.57	0.42
1:A:832:LEU:C	1:A:833:MSE:HG2	2.40	0.42
2:D:1028:PHE:CE2	2:D:1160:LEU:HD23	2.55	0.42
1:C:1664:ASN:ND2	1:C:1664:ASN:C	2.73	0.42
1:A:680:ASN:HD22	1:A:680:ASN:N	2.18	0.42
1:C:1873:CYS:HB3	1:C:1889:TYR:HB3	2.01	0.42
1:A:685:ASN:ND2	1:A:685:ASN:N	2.67	0.41
2:D:1032:TYR:O	2:D:1034:PRO:HD3	2.20	0.41
1:C:1772:ILE:HG13	1:C:1806:LEU:CD2	2.49	0.41
1:C:1909:ASP:OD1	1:C:1911:LYS:HG2	2.20	0.41
1:A:732:LYS:N	1:A:733:PRO:HD2	2.33	0.41
2:D:1113:VAL:HA	2:D:1155:VAL:O	2.20	0.41
1:C:1834:GLN:HA	1:C:1863:LEU:O	2.21	0.41
2:B:184:LYS:HE2	2:B:186:ARG:NH1	2.36	0.41
1:C:1897:MSE:C	1:C:1948:GLN:HE22	2.24	0.41
2:B:147:ARG:CB	2:B:147:ARG:HH11	2.24	0.41
1:C:1681:ILE:HG23	1:C:1734:ARG:HG2	2.03	0.40
2:D:1044:VAL:HG12	2:D:1046:ILE:HD12	2.03	0.40
1:A:709:GLU:H	1:A:709:GLU:CD	2.25	0.40
1:A:654:VAL:HG21	1:A:764:TYR:CB	2.51	0.40
1:A:897:MSE:C	1:A:948:GLN:HE22	2.24	0.40
1:A:914:GLU:OE1	1:A:920:ARG:NH2	2.55	0.40
1:C:1707:CYS:SG	1:C:1710:LEU:HG	2.62	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%)	323 (97%)	7 (2%)	3 (1%)	21 30
1	C	326/353 (92%)	307 (94%)	17 (5%)	2 (1%)	30 43
2	B	186/188 (99%)	175 (94%)	10 (5%)	1 (0%)	34 48
2	D	175/188 (93%)	167 (95%)	8 (5%)	0	100 100
All	All	1020/1082 (94%)	972 (95%)	42 (4%)	6 (1%)	30 43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	ALA
1	A	883	TYR
1	A	963	GLN
1	C	1877	GLU
1	C	1884	GLU
2	B	131	LYS

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	300/304 (99%)	291 (97%)	9 (3%)	48 70
1	C	290/304 (95%)	282 (97%)	8 (3%)	51 72
2	B	168/168 (100%)	167 (99%)	1 (1%)	90 96
2	D	157/168 (94%)	157 (100%)	0	100 100
All	All	915/944 (97%)	897 (98%)	18 (2%)	63 81

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

Mol	Chain	Res	Type
1	A	664	ASN
1	A	680	ASN
1	A	685	ASN
1	A	776	GLN
1	A	790	GLU

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Mol	Chain	Res	Type
1	A	855	ARG
1	A	865	LEU
1	A	893	GLN
1	A	962	GLU
2	B	95	GLU
1	C	1641	LEU
1	C	1654	VAL
1	C	1664	ASN
1	C	1685	ASN
1	C	1744	ASP
1	C	1865	LEU
1	C	1893	GLN
1	C	1916	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	694	ASN
1	A	731	ASN
1	A	843	HIS
1	A	860	GLN
1	A	893	GLN
1	A	948	GLN
2	B	116	GLN
1	C	1664	ASN
1	C	1677	ASN
1	C	1685	ASN
1	C	1694	ASN
1	C	1731	ASN
1	C	1788	HIS
1	C	1843	HIS
1	C	1879	ASN
1	C	1893	GLN
1	C	1948	GLN
2	D	1116	GLN
2	D	1134	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	327/353 (92%)	0.14	24 (7%) 18 18	20, 37, 81, 124	0
1	C	320/353 (90%)	0.24	27 (8%) 14 13	21, 38, 86, 117	0
2	B	188/188 (100%)	-0.20	5 (2%) 58 57	18, 29, 65, 82	0
2	D	177/188 (94%)	0.47	23 (12%) 5 4	22, 43, 89, 98	0
All	All	1012/1082 (93%)	0.17	79 (7%) 16 15	18, 38, 83, 124	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1883	TYR	11.0
1	A	880	GLY	10.4
2	D	1001	MET	9.6
1	A	879	ASN	8.0
1	A	883	TYR	7.7
1	A	881	GLU	7.4
1	A	963	GLN	6.7
1	A	882	GLY	6.3
1	C	1960	ALA	6.2
1	A	959	ARG	6.1
1	C	1884	GLU	5.8
1	C	1879	ASN	5.7
1	C	1882	GLY	5.4
1	A	961	LEU	5.1
1	C	1959	ARG	5.1
1	C	1953	ARG	5.0
1	C	1881	GLU	4.9
1	C	1880	GLY	4.7
1	A	845	LYS	4.6
2	D	1126	ILE	4.5
1	A	844	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	965	HIS	4.4
1	A	960	ALA	4.4
2	D	1130	ALA	4.2
1	A	884	GLU	4.0
1	A	962	GLU	3.8
1	A	964	SER	3.7
2	D	1131	LYS	3.7
2	D	1125	THR	3.7
1	C	1955	ALA	3.6
1	A	877	GLU	3.6
1	A	878	GLU	3.5
2	D	1127	GLU	3.4
1	C	1878	GLU	3.3
1	C	1857	LYS	3.3
1	C	1844	LYS	3.2
2	B	180	PRO	3.1
2	D	1133	LYS	3.1
1	C	1877	GLU	3.0
1	C	1855	ARG	3.0
2	D	1121	ASP	3.0
1	C	1842	ASP	2.9
1	A	876	ARG	2.9
1	C	1954	GLU	2.9
2	D	1123	PRO	2.9
1	C	1910	THR	2.8
2	D	1080	VAL	2.8
2	D	1132	ASN	2.8
2	B	133	LYS	2.7
1	C	1824	ASN	2.7
2	D	1027	LYS	2.7
1	A	846	GLY	2.7
1	A	956	SER	2.6
1	C	1852	GLU	2.6
2	B	130	ALA	2.6
2	D	1002	GLN	2.6
1	C	1921	GLU	2.5
2	D	1107	LYS	2.5
2	B	181	GLU	2.5
2	D	1122	ASP	2.5
1	A	955	ALA	2.4
1	A	790	GLU	2.4
1	C	1756	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	1081	CYS	2.3
2	B	188	SER	2.3
2	D	1129	LEU	2.3
1	C	1841	THR	2.2
2	D	1087	PRO	2.2
2	D	1079	LEU	2.2
2	D	1008	VAL	2.2
1	A	822	ASP	2.2
1	C	1907	LYS	2.1
2	D	1147	ARG	2.1
1	C	1856	PHE	2.1
2	D	1031	GLU	2.1
1	C	1766	LEU	2.1
2	D	1058	THR	2.1
1	A	958	HIS	2.1
1	C	1952	CYS	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 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.