



# Full wwPDB X-ray Structure Validation Report

May 22, 2020 – 05:05 am BST

PDB ID : 5Y3B  
Title : Crystal structure of mouse Ccd1 DIX domain  
Authors : Terawaki, S.; Shibata, N.; Higuchi, Y.  
Deposited on : 2017-07-28  
Resolution : 3.00 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](mailto: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.

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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 : 2.11  
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) : 2.11

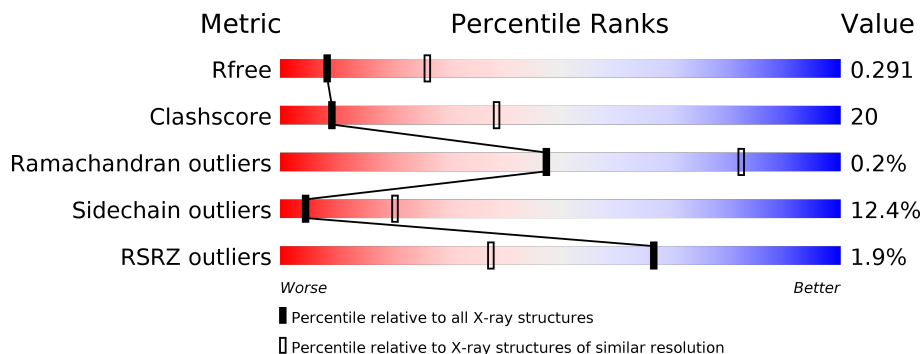
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	86	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 58% 28% 9% 5%</p>
1	B	86	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 51% 37% 6% 6%</p>
1	C	86	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 52% 38% 6% •</p>
1	D	86	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 56% 36% • 6%</p>
1	E	86	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 59% 29% 7% 5%</p>
1	F	86	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 55% 35% 8% •</p>

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Mol	Chain	Length	Quality of chain
1	G	86	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments: a small red segment (5%), a large green segment (52%), a yellow segment (36%), a small orange segment (7%), and a very small grey segment (5%).</p>

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 4664 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 Dixin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	82	668	430	111	125	2	0	0	0
1	B	81	663	427	110	124	2	0	0	0
1	C	83	666	429	112	123	2	0	0	0
1	D	81	661	426	110	123	2	0	0	0
1	E	82	666	429	111	124	2	0	0	0
1	F	84	674	434	113	125	2	0	0	0
1	G	82	666	429	111	124	2	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	GLY	-	expression tag	UNP Q80Y83
A	386	PRO	-	expression tag	UNP Q80Y83
A	387	GLY	-	expression tag	UNP Q80Y83
B	385	GLY	-	expression tag	UNP Q80Y83
B	386	PRO	-	expression tag	UNP Q80Y83
B	387	GLY	-	expression tag	UNP Q80Y83
C	385	GLY	-	expression tag	UNP Q80Y83
C	386	PRO	-	expression tag	UNP Q80Y83
C	387	GLY	-	expression tag	UNP Q80Y83
D	385	GLY	-	expression tag	UNP Q80Y83
D	386	PRO	-	expression tag	UNP Q80Y83
D	387	GLY	-	expression tag	UNP Q80Y83
E	385	GLY	-	expression tag	UNP Q80Y83
E	386	PRO	-	expression tag	UNP Q80Y83
E	387	GLY	-	expression tag	UNP Q80Y83

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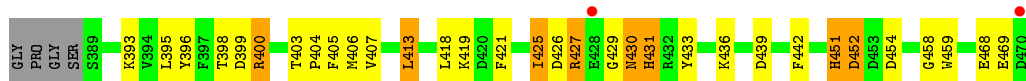
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
F	385	GLY	-	expression tag	UNP Q80Y83
F	386	PRO	-	expression tag	UNP Q80Y83
F	387	GLY	-	expression tag	UNP Q80Y83
G	385	GLY	-	expression tag	UNP Q80Y83
G	386	PRO	-	expression tag	UNP Q80Y83
G	387	GLY	-	expression tag	UNP Q80Y83

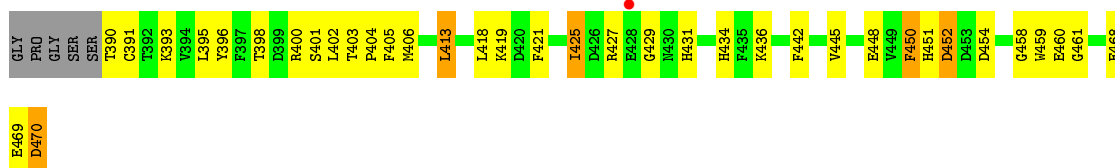
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

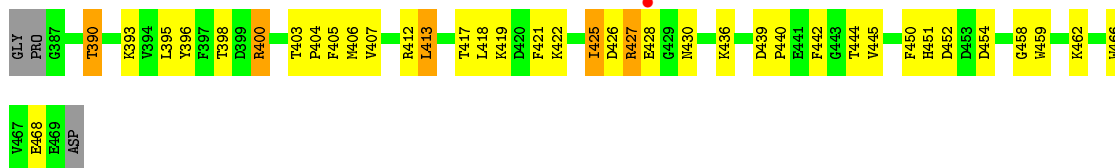
- Molecule 1: Dixin



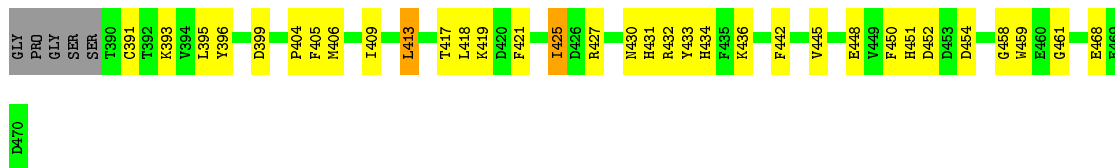
- Molecule 1: Dixin



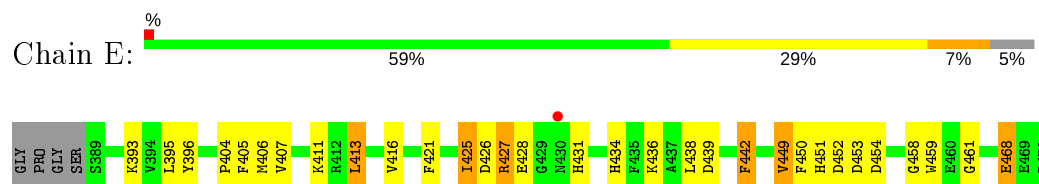
- Molecule 1: Dixin



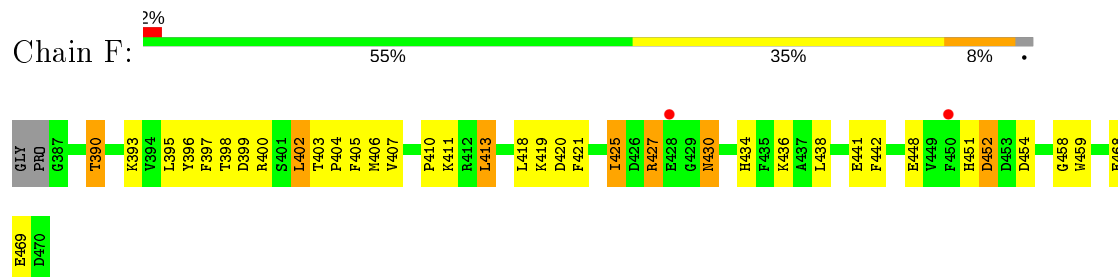
- Molecule 1: Dixin



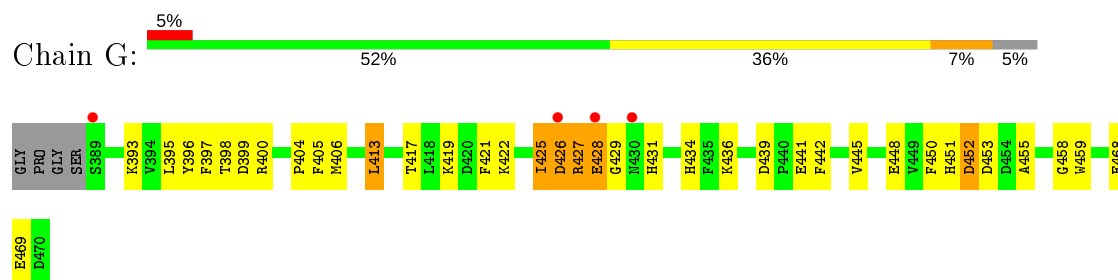
- Molecule 1: Dixin



- Molecule 1: Dixin



- Molecule 1: Dixin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.85Å 75.66Å 125.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 3.00 48.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.09-3.00) 98.4 (48.42-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, $R_{free}$	0.247 , 0.289 0.240 , 0.291	Depositor DCC
$R_{free}$ test set	785 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.24	0/686	0.42	0/929
1	B	0.24	0/681	0.47	0/922
1	C	0.24	0/684	0.43	0/926
1	D	0.22	0/679	0.42	0/919
1	E	0.24	0/684	0.45	0/925
1	F	0.28	0/692	0.47	0/937
1	G	0.23	0/684	0.46	0/926
All	All	0.24	0/4790	0.45	0/6484

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	449	VAL	Peptide

### 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	668	0	640	26	0
1	B	663	0	638	35	0
1	C	666	0	640	33	0
1	D	661	0	633	23	0
1	E	666	0	638	23	0
1	F	674	0	643	25	0
1	G	666	0	641	37	0
All	All	4664	0	4473	182	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 20.

All (182) 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:G:427:ARG:HH11	1:G:427:ARG:HG2	1.07	1.13
1:B:419:LYS:HB2	1:B:452:ASP:HB3	1.45	0.97
1:C:419:LYS:HB2	1:C:452:ASP:HB3	1.54	0.89
1:G:427:ARG:NH1	1:G:427:ARG:HG2	1.80	0.88
1:B:450:PHE:HD1	1:B:450:PHE:H	1.17	0.88
1:G:427:ARG:HH11	1:G:427:ARG:CG	1.88	0.86
1:C:407:VAL:HG12	1:D:448:GLU:HB3	1.57	0.86
1:G:422:LYS:HB3	1:G:427:ARG:HG3	1.60	0.82
1:F:390:THR:O	1:F:410:PRO:O	1.98	0.80
1:F:427:ARG:HD3	1:F:427:ARG:H	1.48	0.79
1:A:419:LYS:HB2	1:A:452:ASP:HB3	1.67	0.76
1:B:450:PHE:N	1:B:450:PHE:CD1	2.52	0.75
1:B:450:PHE:HD1	1:B:450:PHE:N	1.83	0.74
1:F:398:THR:HG22	1:F:400:ARG:H	1.52	0.74
1:B:469:GLU:O	1:B:470:ASP:HB2	1.88	0.73
1:C:468:GLU:HG2	1:F:402:LEU:HD13	1.69	0.72
1:E:426:ASP:OD2	1:E:431:HIS:HD2	1.72	0.72
1:D:419:LYS:HB2	1:D:452:ASP:HB3	1.72	0.71
1:B:395:LEU:HD22	1:C:442:PHE:CG	2.28	0.69
1:B:421:PHE:O	1:B:425:ILE:HG12	1.93	0.68
1:F:419:LYS:HB2	1:F:452:ASP:HB3	1.75	0.67
1:G:434:HIS:HD2	1:G:468:GLU:OE2	1.79	0.66
1:A:407:VAL:HG12	1:B:448:GLU:HB3	1.76	0.66
1:E:434:HIS:HD2	1:E:468:GLU:OE2	1.78	0.66
1:A:418:LEU:HB3	1:A:452:ASP:HA	1.78	0.65
1:G:428:GLU:N	1:G:429:GLY:HA3	2.11	0.64
1:C:422:LYS:HB3	1:C:427:ARG:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:ARG:HD2	1:E:427:ARG:H	1.63	0.63
1:E:421:PHE:O	1:E:425:ILE:HD13	1.98	0.63
1:G:434:HIS:CD2	1:G:468:GLU:OE2	2.53	0.62
1:G:427:ARG:C	1:G:429:GLY:HA3	2.20	0.61
1:F:404:PRO:O	1:G:445:VAL:HG23	1.99	0.61
1:B:413:LEU:HD12	1:B:461:GLY:HA2	1.83	0.61
1:E:395:LEU:HD22	1:F:442:PHE:CD2	2.35	0.61
1:F:427:ARG:HD3	1:F:427:ARG:N	2.14	0.61
1:D:418:LEU:HB3	1:D:452:ASP:HA	1.82	0.60
1:G:422:LYS:HB3	1:G:427:ARG:CG	2.31	0.60
1:C:404:PRO:O	1:D:445:VAL:HG23	2.02	0.60
1:C:418:LEU:HB3	1:C:452:ASP:HA	1.84	0.59
1:E:451:HIS:HB2	1:E:454:ASP:CG	2.22	0.59
1:G:419:LYS:HE3	1:G:452:ASP:HB3	1.84	0.59
1:D:434:HIS:CD2	1:D:468:GLU:OE2	2.54	0.59
1:C:396:TYR:CZ	1:C:425:ILE:HG22	2.38	0.59
1:D:451:HIS:HB2	1:D:454:ASP:OD1	2.03	0.59
1:B:395:LEU:HD22	1:C:442:PHE:CD2	2.38	0.58
1:C:417:THR:HB	1:C:452:ASP:O	2.03	0.58
1:G:400:ARG:HB2	1:G:400:ARG:HH11	1.67	0.58
1:B:418:LEU:HB3	1:B:452:ASP:HA	1.86	0.57
1:B:393:LYS:HE2	1:B:406:MET:SD	2.45	0.57
1:D:393:LYS:HE2	1:D:406:MET:SD	2.44	0.57
1:A:431:HIS:HB3	1:A:468:GLU:O	2.05	0.57
1:G:427:ARG:N	1:G:427:ARG:HD3	2.20	0.56
1:A:393:LYS:HE2	1:A:406:MET:SD	2.45	0.56
1:C:390:THR:HG23	1:C:412:ARG:HH21	1.70	0.56
1:G:421:PHE:O	1:G:425:ILE:HD13	2.04	0.56
1:E:393:LYS:HE2	1:E:406:MET:SD	2.45	0.56
1:C:393:LYS:HE2	1:C:406:MET:SD	2.46	0.56
1:G:393:LYS:HE2	1:G:406:MET:SD	2.46	0.55
1:E:434:HIS:CD2	1:E:468:GLU:OE2	2.60	0.55
1:F:393:LYS:HE2	1:F:406:MET:SD	2.46	0.55
1:D:434:HIS:HD2	1:D:468:GLU:OE2	1.91	0.54
1:F:407:VAL:HG12	1:G:448:GLU:HB3	1.89	0.54
1:D:413:LEU:HD21	1:D:458:GLY:HA3	1.89	0.54
1:G:428:GLU:N	1:G:429:GLY:CA	2.70	0.54
1:C:426:ASP:HB2	1:D:432:ARG:NH2	2.23	0.53
1:A:413:LEU:HD21	1:A:458:GLY:HA3	1.90	0.53
1:E:449:VAL:CG1	1:E:450:PHE:H	2.21	0.53
1:E:413:LEU:HD21	1:E:458:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:PHE:CZ	1:D:425:ILE:HD11	2.44	0.53
1:G:413:LEU:HD21	1:G:458:GLY:HA3	1.90	0.53
1:G:400:ARG:NH1	1:G:400:ARG:HB2	2.23	0.53
1:C:439:ASP:CG	1:C:440:PRO:HD2	2.29	0.53
1:B:425:ILE:HG22	1:B:427:ARG:NH1	2.24	0.53
1:D:431:HIS:HB2	1:D:433:TYR:CZ	2.44	0.53
1:F:413:LEU:HD21	1:F:458:GLY:HA3	1.90	0.53
1:C:413:LEU:HD21	1:C:458:GLY:HA3	1.90	0.52
1:B:413:LEU:HD21	1:B:458:GLY:HA3	1.90	0.52
1:B:459:TRP:O	1:B:460:GLU:HB2	2.09	0.52
1:D:395:LEU:HD11	1:D:404:PRO:HB2	1.92	0.52
1:E:421:PHE:CE1	1:E:425:ILE:HD11	2.45	0.52
1:G:398:THR:HG22	1:G:400:ARG:H	1.74	0.52
1:G:395:LEU:HD11	1:G:404:PRO:HB2	1.92	0.52
1:G:431:HIS:HB3	1:G:468:GLU:O	2.10	0.52
1:B:419:LYS:HE3	1:B:452:ASP:HB3	1.91	0.51
1:A:395:LEU:HD11	1:A:404:PRO:HB2	1.92	0.51
1:F:395:LEU:HD22	1:G:442:PHE:CD2	2.46	0.51
1:C:395:LEU:HD22	1:D:442:PHE:CG	2.45	0.51
1:F:411:LYS:HE2	1:F:420:ASP:OD2	2.10	0.51
1:C:395:LEU:HD11	1:C:404:PRO:HB2	1.93	0.51
1:A:430:ASN:N	1:A:430:ASN:OD1	2.43	0.51
1:B:434:HIS:CD2	1:B:468:GLU:OE2	2.63	0.51
1:F:395:LEU:HD11	1:F:404:PRO:HB2	1.92	0.51
1:G:398:THR:HG22	1:G:399:ASP:N	2.25	0.51
1:A:395:LEU:HD22	1:B:442:PHE:CD1	2.46	0.50
1:A:427:ARG:HB2	1:A:431:HIS:NE2	2.26	0.50
1:A:427:ARG:CZ	1:A:429:GLY:O	2.60	0.50
1:B:401:SER:O	1:B:402:LEU:HB2	2.12	0.50
1:F:421:PHE:O	1:F:425:ILE:HD13	2.12	0.50
1:B:395:LEU:HD11	1:B:404:PRO:HB2	1.92	0.50
1:C:419:LYS:HE3	1:C:452:ASP:HB3	1.94	0.49
1:C:396:TYR:CZ	1:C:425:ILE:CG2	2.95	0.49
1:B:429:GLY:HA3	1:B:431:HIS:NE2	2.27	0.49
1:C:398:THR:HG22	1:C:400:ARG:H	1.78	0.49
1:D:413:LEU:HD12	1:D:461:GLY:HA2	1.94	0.49
1:F:418:LEU:HB3	1:F:452:ASP:HA	1.94	0.49
1:A:398:THR:HG22	1:A:400:ARG:H	1.77	0.49
1:E:395:LEU:HD11	1:E:404:PRO:HB2	1.93	0.49
1:E:426:ASP:OD2	1:E:431:HIS:CD2	2.60	0.49
1:F:451:HIS:HB2	1:F:454:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:PHE:O	1:D:425:ILE:HG12	2.13	0.48
1:B:425:ILE:HG22	1:B:427:ARG:HH11	1.78	0.48
1:E:427:ARG:CD	1:E:427:ARG:H	2.22	0.48
1:G:439:ASP:OD2	1:G:441:GLU:HB2	2.14	0.48
1:B:390:THR:HG23	1:B:391:CYS:H	1.78	0.47
1:A:404:PRO:O	1:B:445:VAL:HG23	2.15	0.47
1:E:449:VAL:CG1	1:E:450:PHE:N	2.77	0.47
1:E:413:LEU:HD12	1:E:461:GLY:HA2	1.96	0.47
1:A:396:TYR:CZ	1:A:425:ILE:HG22	2.49	0.47
1:C:451:HIS:HB2	1:C:454:ASP:CG	2.35	0.47
1:G:417:THR:HA	1:G:455:ALA:HA	1.96	0.47
1:C:422:LYS:HD3	1:C:427:ARG:HH11	1.80	0.47
1:A:431:HIS:HD2	1:A:433:TYR:OH	1.99	0.46
1:A:451:HIS:N	1:A:451:HIS:ND1	2.63	0.46
1:B:425:ILE:H	1:B:425:ILE:HG12	1.16	0.46
1:G:421:PHE:CE1	1:G:425:ILE:HD11	2.51	0.46
1:C:436:LYS:HE2	1:C:459:TRP:CE2	2.51	0.46
1:B:421:PHE:O	1:B:425:ILE:CG1	2.62	0.46
1:D:391:CYS:HB2	1:D:409:ILE:O	2.16	0.46
1:G:427:ARG:O	1:G:427:ARG:CZ	2.64	0.46
1:C:421:PHE:CD1	1:C:425:ILE:HD11	2.51	0.46
1:A:436:LYS:HE2	1:A:459:TRP:CE2	2.51	0.45
1:G:436:LYS:HE2	1:G:459:TRP:CE2	2.52	0.45
1:A:421:PHE:CE1	1:A:425:ILE:HD11	2.51	0.45
1:A:427:ARG:HD2	1:A:433:TYR:OH	2.16	0.45
1:E:407:VAL:HG12	1:F:448:GLU:HB3	1.98	0.45
1:E:436:LYS:HE2	1:E:459:TRP:CE2	2.51	0.45
1:E:439:ASP:OD2	1:E:442:PHE:CD2	2.70	0.45
1:D:436:LYS:HE2	1:D:459:TRP:CE2	2.51	0.45
1:B:401:SER:O	1:B:402:LEU:CB	2.64	0.45
1:B:436:LYS:HE2	1:B:459:TRP:CE2	2.52	0.44
1:G:425:ILE:O	1:G:426:ASP:C	2.55	0.44
1:F:436:LYS:HE2	1:F:459:TRP:CE2	2.52	0.44
1:G:450:PHE:CE2	1:G:451:HIS:CE1	3.05	0.44
1:E:449:VAL:HG12	1:E:450:PHE:N	2.32	0.44
1:F:396:TYR:CZ	1:F:405:PHE:HB2	2.53	0.44
1:A:439:ASP:OD1	1:A:442:PHE:N	2.39	0.44
1:G:426:ASP:O	1:G:427:ARG:C	2.55	0.44
1:C:396:TYR:CZ	1:C:405:PHE:HB2	2.53	0.44
1:C:417:THR:HA	1:C:454:ASP:O	2.18	0.44
1:E:438:LEU:O	1:E:438:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:TYR:CZ	1:G:405:PHE:HB2	2.53	0.44
1:A:396:TYR:CZ	1:A:405:PHE:HB2	2.53	0.44
1:F:434:HIS:CD2	1:F:468:GLU:OE2	2.71	0.44
1:A:400:ARG:HH11	1:A:400:ARG:HB3	1.83	0.43
1:A:431:HIS:CD2	1:A:431:HIS:N	2.86	0.43
1:B:398:THR:C	1:B:400:ARG:H	2.22	0.43
1:G:396:TYR:CZ	1:G:425:ILE:HG21	2.53	0.43
1:D:396:TYR:CZ	1:D:405:PHE:HB2	2.53	0.43
1:B:469:GLU:O	1:B:470:ASP:CB	2.61	0.43
1:E:396:TYR:CZ	1:E:405:PHE:HB2	2.53	0.42
1:A:439:ASP:OD1	1:A:442:PHE:CD2	2.72	0.42
1:B:396:TYR:CZ	1:B:405:PHE:HB2	2.54	0.42
1:B:401:SER:C	1:B:403:THR:H	2.23	0.42
1:E:411:LYS:HB2	1:E:416:VAL:HG22	2.02	0.42
1:C:466:TRP:HB3	1:F:402:LEU:HD11	2.02	0.42
1:C:439:ASP:HA	1:C:440:PRO:HD3	1.85	0.42
1:C:400:ARG:HG2	1:G:397:PHE:CE1	2.55	0.42
1:G:398:THR:HG22	1:G:400:ARG:N	2.35	0.42
1:D:417:THR:HB	1:D:452:ASP:O	2.19	0.41
1:C:421:PHE:O	1:C:425:ILE:CD1	2.69	0.41
1:A:451:HIS:HB2	1:A:454:ASP:OD1	2.21	0.41
1:B:419:LYS:HE3	1:B:452:ASP:CB	2.50	0.41
1:B:451:HIS:HB2	1:B:454:ASP:OD1	2.20	0.41
1:B:406:MET:HB2	1:C:445:VAL:HG21	2.02	0.41
1:D:425:ILE:HG12	1:D:425:ILE:H	1.51	0.41
1:D:413:LEU:HD21	1:D:458:GLY:CA	2.51	0.41
1:C:426:ASP:CB	1:D:432:ARG:NH2	2.84	0.41
1:F:395:LEU:HD22	1:G:442:PHE:CG	2.55	0.41
1:A:413:LEU:HD21	1:A:458:GLY:CA	2.51	0.41
1:F:430:ASN:N	1:F:430:ASN:OD1	2.54	0.40
1:C:422:LYS:HD3	1:C:427:ARG:NH1	2.37	0.40
1:F:397:PHE:CE1	1:F:404:PRO:HB3	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
1	B	79/86 (92%)	71 (90%)	8 (10%)	0	100	100
1	C	81/86 (94%)	77 (95%)	4 (5%)	0	100	100
1	D	79/86 (92%)	75 (95%)	4 (5%)	0	100	100
1	E	80/86 (93%)	73 (91%)	7 (9%)	0	100	100
1	F	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
1	G	80/86 (93%)	75 (94%)	4 (5%)	1 (1%)	12	45
All	All	561/602 (93%)	524 (93%)	36 (6%)	1 (0%)	47	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	426	ASP

### 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	71/74 (96%)	59 (83%)	12 (17%)	2	11
1	B	71/74 (96%)	66 (93%)	5 (7%)	15	47
1	C	70/74 (95%)	59 (84%)	11 (16%)	2	13
1	D	70/74 (95%)	64 (91%)	6 (9%)	10	37
1	E	70/74 (95%)	62 (89%)	8 (11%)	5	24
1	F	70/74 (95%)	58 (83%)	12 (17%)	2	10
1	G	71/74 (96%)	64 (90%)	7 (10%)	8	30
All	All	493/518 (95%)	432 (88%)	61 (12%)	4	20

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	ASP
1	A	400	ARG
1	A	403	THR
1	A	413	LEU
1	A	425	ILE
1	A	426	ASP
1	A	427	ARG
1	A	430	ASN
1	A	431	HIS
1	A	451	HIS
1	A	452	ASP
1	A	469	GLU
1	B	413	LEU
1	B	425	ILE
1	B	450	PHE
1	B	452	ASP
1	B	470	ASP
1	C	390	THR
1	C	400	ARG
1	C	403	THR
1	C	413	LEU
1	C	425	ILE
1	C	427	ARG
1	C	428	GLU
1	C	430	ASN
1	C	444	THR
1	C	450	PHE
1	C	462	LYS
1	D	399	ASP
1	D	413	LEU
1	D	425	ILE
1	D	427	ARG
1	D	430	ASN
1	D	450	PHE
1	E	413	LEU
1	E	425	ILE
1	E	427	ARG
1	E	428	GLU
1	E	442	PHE
1	E	452	ASP
1	E	453	ASP
1	E	468	GLU
1	F	390	THR

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Mol	Chain	Res	Type
1	F	399	ASP
1	F	402	LEU
1	F	403	THR
1	F	413	LEU
1	F	425	ILE
1	F	427	ARG
1	F	430	ASN
1	F	438	LEU
1	F	441	GLU
1	F	452	ASP
1	F	469	GLU
1	G	413	LEU
1	G	425	ILE
1	G	427	ARG
1	G	428	GLU
1	G	452	ASP
1	G	453	ASP
1	G	469	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	HIS
1	B	434	HIS
1	D	434	HIS
1	E	431	HIS
1	E	434	HIS
1	F	434	HIS
1	G	434	HIS
1	G	451	HIS

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	82/86 (95%)	-0.13	2 (2%) 59 30	20, 56, 104, 151	0
1	B	81/86 (94%)	-0.18	1 (1%) 79 54	19, 53, 116, 174	0
1	C	83/86 (96%)	-0.23	1 (1%) 79 54	21, 52, 112, 173	0
1	D	81/86 (94%)	-0.27	0 100 100	18, 50, 95, 118	0
1	E	82/86 (95%)	-0.04	1 (1%) 79 54	18, 54, 98, 136	0
1	F	84/86 (97%)	-0.27	2 (2%) 59 30	20, 51, 108, 147	0
1	G	82/86 (95%)	-0.02	4 (4%) 29 11	21, 58, 131, 151	0
All	All	575/602 (95%)	-0.16	11 (1%) 66 37	18, 53, 113, 174	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	GLU	3.6
1	B	428	GLU	3.0
1	G	389	SER	2.9
1	A	470	ASP	2.7
1	C	428	GLU	2.6
1	G	428	GLU	2.3
1	G	430	ASN	2.3
1	E	430	ASN	2.2
1	F	450	PHE	2.2
1	G	426	ASP	2.1
1	F	428	GLU	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.