



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 05:27 PM EDT

PDB ID : 3SF4  
Title : Crystal structure of the complex between the conserved cell polarity proteins  
Inscuteable and LGN  
Authors : Yuzawa, S.; Kamakura, S.; Iwakiri, Y.; Hayase, J.; Sumimoto, H.  
Deposited on : 2011-06-12  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

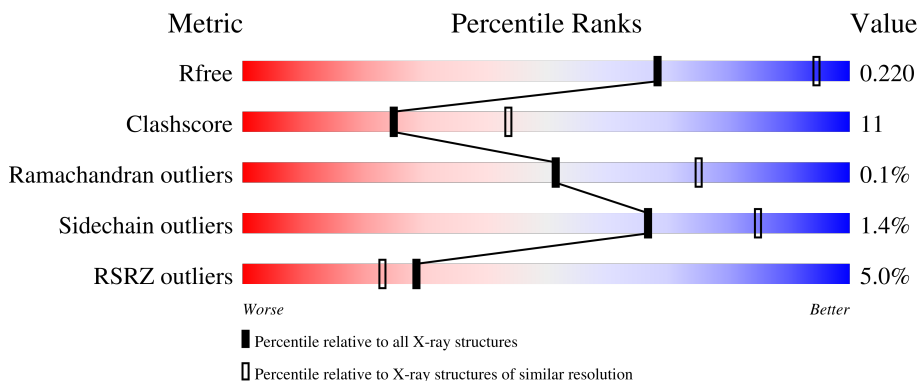
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



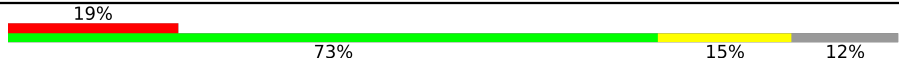
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of 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	406	 73% 14% 13%
1	B	406	 7% 65% 21% 14%
1	C	406	 67% 18% 15%
2	D	52	 15% 63% 23% 13%
2	E	52	 8% 60% 19% 21%

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Mol	Chain	Length	Quality of chain
2	F	52	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '19%', a large green segment labeled '73%', a yellow segment labeled '15%', and a grey segment on the far right labeled '12%'.</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9330 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 G-protein-signaling modulator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	Total	C	N	O	S	0	0	0
			2759	1729	487	534	9			
1	B	350	Total	C	N	O	S	0	0	0
			2691	1685	474	524	8			
1	C	346	Total	C	N	O	S	0	0	0
			2687	1681	474	523	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	EXPRESSION TAG	UNP P81274
A	10	PRO	-	EXPRESSION TAG	UNP P81274
A	11	GLY	-	EXPRESSION TAG	UNP P81274
A	12	SER	-	EXPRESSION TAG	UNP P81274
B	9	GLY	-	EXPRESSION TAG	UNP P81274
B	10	PRO	-	EXPRESSION TAG	UNP P81274
B	11	GLY	-	EXPRESSION TAG	UNP P81274
B	12	SER	-	EXPRESSION TAG	UNP P81274
C	9	GLY	-	EXPRESSION TAG	UNP P81274
C	10	PRO	-	EXPRESSION TAG	UNP P81274
C	11	GLY	-	EXPRESSION TAG	UNP P81274
C	12	SER	-	EXPRESSION TAG	UNP P81274

- Molecule 2 is a protein called Protein inscuteable homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	45	Total	C	N	O	S	0	0	0
			343	212	55	70	6			
2	E	41	Total	C	N	O	S	0	0	0
			302	189	50	57	6			
2	F	46	Total	C	N	O	S	0	0	0
			340	211	55	68	6			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	18	GLY	-	EXPRESSION TAG	UNP Q1MX18
D	19	PRO	-	EXPRESSION TAG	UNP Q1MX18
D	20	LEU	-	EXPRESSION TAG	UNP Q1MX18
D	21	GLY	-	EXPRESSION TAG	UNP Q1MX18
D	22	SER	-	EXPRESSION TAG	UNP Q1MX18
E	18	GLY	-	EXPRESSION TAG	UNP Q1MX18
E	19	PRO	-	EXPRESSION TAG	UNP Q1MX18
E	20	LEU	-	EXPRESSION TAG	UNP Q1MX18
E	21	GLY	-	EXPRESSION TAG	UNP Q1MX18
E	22	SER	-	EXPRESSION TAG	UNP Q1MX18
F	18	GLY	-	EXPRESSION TAG	UNP Q1MX18
F	19	PRO	-	EXPRESSION TAG	UNP Q1MX18
F	20	LEU	-	EXPRESSION TAG	UNP Q1MX18
F	21	GLY	-	EXPRESSION TAG	UNP Q1MX18
F	22	SER	-	EXPRESSION TAG	UNP Q1MX18

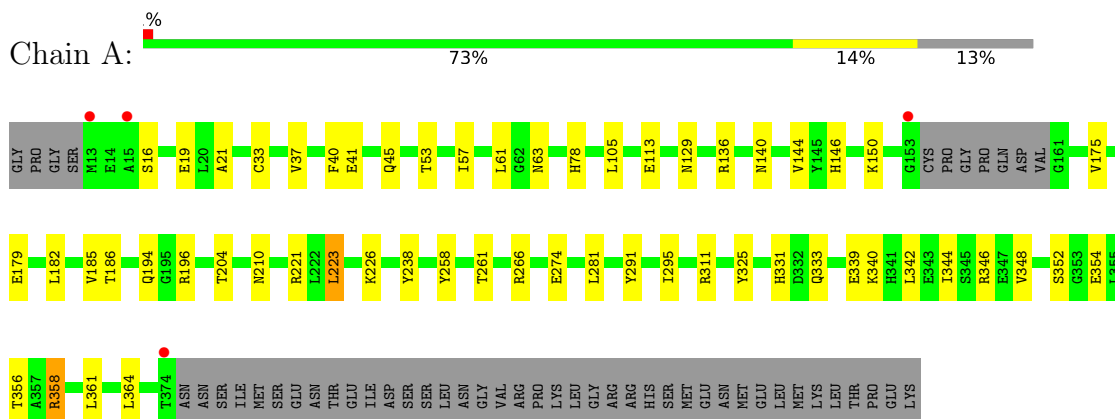
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	49	Total O 49 49	0	0
3	C	60	Total O 60 60	0	0
3	D	7	Total O 7 7	0	0
3	E	4	Total O 4 4	0	0
3	F	11	Total O 11 11	0	0

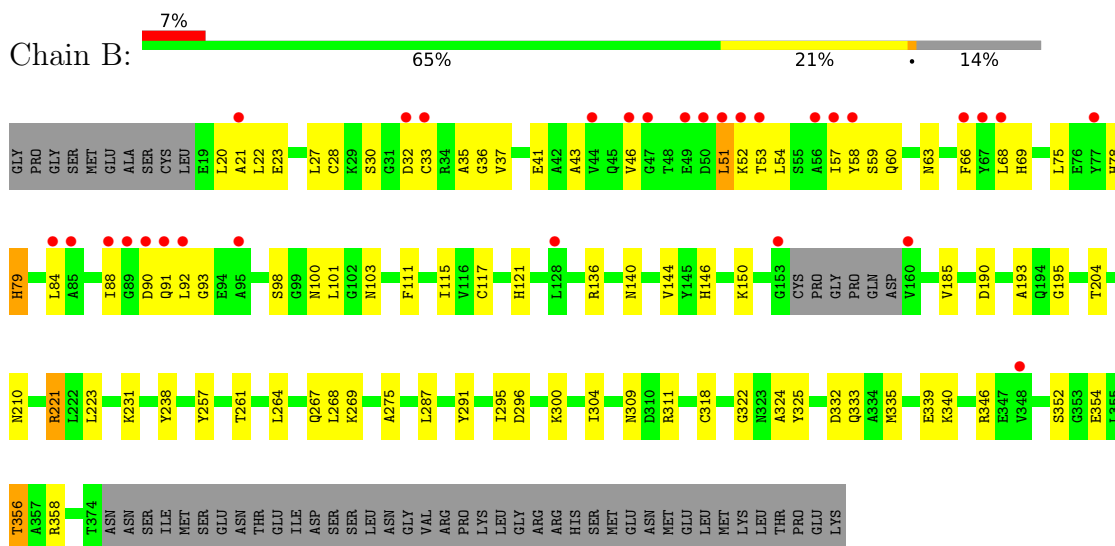
### 3 Residue-property plots [i](#)

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

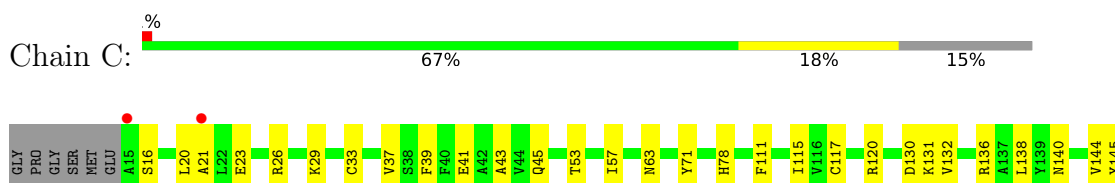
- Molecule 1: G-protein-signaling modulator 2

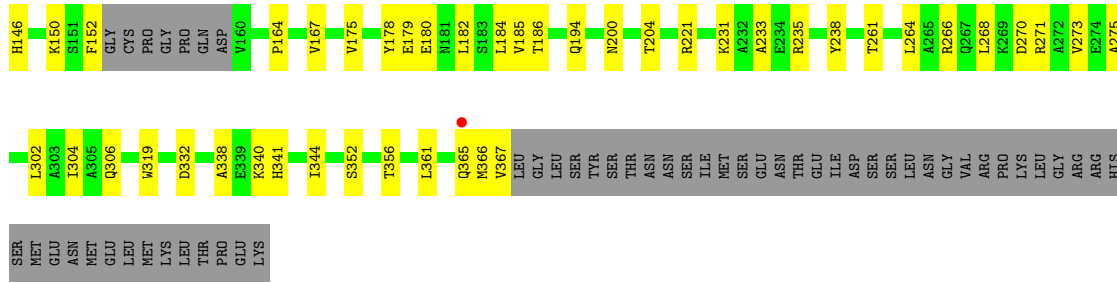


- Molecule 1: G-protein-signaling modulator 2

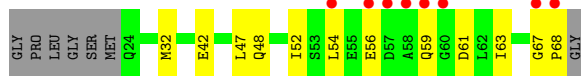


- Molecule 1: G-protein-signaling modulator 2





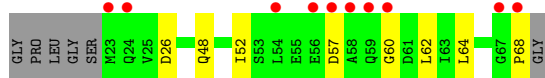
• Molecule 2: Protein in-scuteable homolog



• Molecule 2: Protein in-scuteable homolog



• Molecule 2: Protein in-scuteable homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.81Å 124.81Å 233.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.60 48.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.72-2.60) 99.9 (48.72-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.216 , 0.262 0.218 , 0.220	Depositor DCC
$R_{free}$ test set	2839 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.35	0/2805	0.52	0/3782
1	B	0.34	0/2736	0.50	0/3695
1	C	0.35	0/2732	0.50	0/3685
2	D	0.35	0/346	0.67	0/466
2	E	0.31	0/304	0.63	0/407
2	F	0.32	0/343	0.65	0/463
All	All	0.35	0/9266	0.53	0/12498

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 [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	2759	0	2668	47	0
1	B	2691	0	2566	75	0
1	C	2687	0	2576	60	0
2	D	343	0	338	14	0
2	E	302	0	300	15	0
2	F	340	0	330	8	0
3	A	77	0	0	2	0
3	B	49	0	0	1	0
3	C	60	0	0	0	0
3	D	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	4	0	0	0	0
3	F	11	0	0	0	0
All	All	9330	0	8778	194	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 (194) 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:136:ARG:HH11	2:F:48:GLN:HE21	1.21	0.89
1:A:182:LEU:O	1:A:186:THR:HG23	1.73	0.86
1:B:27:LEU:HD13	1:B:36:GLY:HA2	1.57	0.86
1:B:287:LEU:HD23	2:E:24:GLN:HE21	1.40	0.84
1:C:182:LEU:O	1:C:186:THR:HG23	1.81	0.79
1:A:291:TYR:O	1:A:295:ILE:HG12	1.83	0.78
1:A:185:VAL:HG12	1:A:194:GLN:HG3	1.67	0.77
1:B:136:ARG:HH11	2:E:48:GLN:HE21	1.32	0.77
1:C:136:ARG:HH11	2:F:48:GLN:NE2	1.85	0.74
1:B:136:ARG:NH1	2:E:48:GLN:HE21	1.85	0.74
1:C:185:VAL:HG12	1:C:194:GLN:HG3	1.68	0.73
1:B:287:LEU:HD23	2:E:24:GLN:NE2	2.03	0.73
1:B:231:LYS:HD2	1:B:264:LEU:HD11	1.70	0.72
1:C:136:ARG:NH1	2:F:48:GLN:HE21	1.88	0.71
1:C:366:MET:HG3	1:C:367:VAL:H	1.56	0.70
1:C:366:MET:HG3	1:C:367:VAL:N	2.04	0.70
1:A:136:ARG:HH11	2:D:48:GLN:HE21	1.39	0.70
1:C:131:LYS:HD2	1:C:184:LEU:HD11	1.74	0.70
1:B:238:TYR:HB2	1:B:261:THR:HG22	1.74	0.69
1:B:51:LEU:HD22	1:B:84:LEU:HD11	1.74	0.69
1:B:136:ARG:HH11	2:E:48:GLN:NE2	1.91	0.68
1:B:52:LYS:HA	1:B:52:LYS:HE2	1.75	0.68
1:A:238:TYR:HB2	1:A:261:THR:HG22	1.76	0.67
1:C:23:GLU:HG2	1:C:39:PHE:CE2	2.30	0.67
1:B:238:TYR:CB	1:B:261:THR:HG22	2.25	0.67
1:B:146:HIS:CE1	1:B:150:LYS:HE3	2.31	0.66
1:C:45:GLN:NE2	1:C:45:GLN:HA	2.10	0.66
2:D:32:MET:CE	2:E:19:PRO:HB3	2.27	0.65
1:B:21:ALA:HB2	1:B:43:ALA:HB2	1.78	0.65
1:C:231:LYS:HD2	1:C:264:LEU:HD11	1.78	0.64
1:C:111:PHE:O	1:C:115:ILE:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HD2	1:A:274:GLU:OE1	1.98	0.64
1:B:21:ALA:HB2	1:B:43:ALA:CB	2.29	0.63
1:C:26:ARG:HB3	1:C:26:ARG:NH1	2.14	0.63
1:C:361:LEU:O	1:C:365:GLN:HG3	1.98	0.62
1:B:20:LEU:HD11	1:B:43:ALA:CA	2.30	0.62
1:B:32:ASP:OD2	1:B:35:ALA:HB3	2.00	0.61
1:B:22:LEU:O	1:B:22:LEU:HD23	1.99	0.61
1:B:53:THR:O	1:B:57:ILE:HG12	1.99	0.61
1:B:346:ARG:HG2	1:B:354:GLU:OE2	2.01	0.60
1:A:186:THR:HA	1:A:194:GLN:NE2	2.17	0.60
1:B:146:HIS:HE1	1:B:150:LYS:HE3	1.67	0.60
1:A:186:THR:HG22	1:A:194:GLN:HG2	1.83	0.60
1:A:33:CYS:O	1:A:37:VAL:HG23	2.02	0.59
1:B:291:TYR:O	1:B:295:ILE:HG12	2.02	0.59
1:B:346:ARG:NH2	1:B:358:ARG:HH22	2.01	0.59
1:C:53:THR:O	1:C:57:ILE:HG12	2.02	0.59
2:D:54:LEU:HD12	2:D:54:LEU:H	1.68	0.59
1:B:54:LEU:HG	1:B:58:TYR:HE2	1.68	0.59
1:B:335:MET:O	1:B:339:GLU:HG3	2.02	0.59
1:C:366:MET:HG3	1:C:367:VAL:HG23	1.85	0.58
1:C:21:ALA:HB1	2:F:52:ILE:HD13	1.85	0.58
1:C:221:ARG:NH2	1:C:233:ALA:HB1	2.19	0.58
1:A:352:SER:O	1:A:356:THR:HG23	2.03	0.58
1:B:20:LEU:HD12	1:B:20:LEU:C	2.24	0.58
1:C:20:LEU:HB2	1:C:43:ALA:HB2	1.85	0.57
1:A:340:LYS:O	1:A:344:ILE:HG12	2.05	0.57
1:C:146:HIS:CE1	1:C:150:LYS:HE3	2.40	0.57
1:B:92:LEU:HD23	1:B:92:LEU:O	2.05	0.57
1:C:340:LYS:O	1:C:344:ILE:HD13	2.03	0.57
1:C:175:VAL:O	1:C:179:GLU:HG3	2.03	0.57
1:C:37:VAL:O	1:C:41:GLU:HG3	2.05	0.56
1:C:238:TYR:HB2	1:C:261:THR:HG22	1.87	0.56
2:E:29:GLN:O	2:E:33:GLU:HG3	2.04	0.56
2:D:32:MET:HE1	2:E:19:PRO:HB3	1.87	0.56
1:C:45:GLN:HA	1:C:45:GLN:HE21	1.71	0.56
1:C:319:TRP:NE1	2:F:26:ASP:OD2	2.39	0.56
1:A:331:HIS:HE1	1:A:364:LEU:O	1.89	0.56
1:A:136:ARG:HH11	2:D:48:GLN:NE2	2.04	0.56
1:B:140:ASN:O	1:B:144:VAL:HG23	2.06	0.56
1:C:275:ALA:HB2	1:C:304:ILE:HG21	1.87	0.56
1:C:238:TYR:CB	1:C:261:THR:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:GLU:HA	2:D:59:GLN:HG2	1.89	0.55
1:A:53:THR:O	1:A:57:ILE:HG12	2.05	0.55
1:B:352:SER:O	1:B:356:THR:HG22	2.07	0.55
1:A:63:ASN:ND2	1:A:78:HIS:CE1	2.74	0.55
1:A:146:HIS:HD2	1:A:204:THR:OG1	1.90	0.54
1:B:63:ASN:ND2	1:B:78:HIS:CE1	2.75	0.54
1:B:20:LEU:HD11	1:B:43:ALA:HA	1.89	0.54
1:A:185:VAL:CG1	1:A:194:GLN:HG3	2.36	0.54
1:B:103:ASN:ND2	2:E:45:CYS:HA	2.23	0.54
2:D:54:LEU:HD12	2:D:54:LEU:N	2.22	0.54
1:C:71:TYR:CZ	2:F:68:PRO:HD3	2.43	0.53
1:B:20:LEU:CD2	1:B:46:VAL:HG21	2.38	0.53
1:C:63:ASN:ND2	1:C:78:HIS:CE1	2.77	0.53
1:B:66:PHE:CD2	2:E:47:LEU:HD11	2.44	0.53
1:B:27:LEU:HD13	1:B:36:GLY:CA	2.36	0.53
1:B:322:GLY:HA3	3:B:443:HOH:O	2.09	0.52
1:B:195:GLY:O	1:B:221:ARG:HD2	2.10	0.52
1:C:235:ARG:O	1:C:235:ARG:HD2	2.09	0.52
1:A:196:ARG:HA	2:D:42:GLU:HG3	1.92	0.52
1:B:90:ASP:OD2	1:B:93:GLY:HA3	2.10	0.51
1:C:302:LEU:O	1:C:306:GLN:HG3	2.11	0.51
1:C:26:ARG:HB3	1:C:26:ARG:HH11	1.76	0.51
1:A:358:ARG:NH1	1:A:358:ARG:O	2.44	0.51
1:A:238:TYR:HB3	1:A:261:THR:HG23	1.92	0.51
1:C:275:ALA:HB2	1:C:304:ILE:CG2	2.41	0.50
2:D:48:GLN:HA	2:D:61:ASP:O	2.12	0.50
1:B:27:LEU:HD23	1:B:27:LEU:O	2.12	0.50
1:C:45:GLN:HE21	1:C:45:GLN:CA	2.23	0.49
1:C:231:LYS:HB3	1:C:268:LEU:HD21	1.95	0.49
1:B:185:VAL:CG1	1:B:193:ALA:HB3	2.43	0.49
1:B:54:LEU:HG	1:B:58:TYR:CE2	2.45	0.49
1:B:257:TYR:O	1:B:261:THR:HG23	2.13	0.49
1:B:295:ILE:HD13	1:B:324:ALA:HB1	1.95	0.48
1:C:238:TYR:HB3	1:C:261:THR:CG2	2.42	0.48
1:A:342:LEU:HD11	1:A:346:ARG:NH1	2.27	0.48
1:B:33:CYS:O	1:B:37:VAL:HG23	2.13	0.48
1:C:146:HIS:HD2	1:C:204:THR:OG1	1.96	0.48
1:A:358:ARG:HH11	1:A:358:ARG:HA	1.79	0.48
1:B:75:LEU:O	1:B:79:HIS:HB2	2.13	0.48
1:B:185:VAL:HG13	1:B:190:ASP:HB3	1.95	0.48
1:C:140:ASN:O	1:C:144:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:TYR:HB3	1:B:261:THR:CG2	2.43	0.48
1:A:346:ARG:HG3	1:A:354:GLU:HG3	1.96	0.48
1:A:238:TYR:CB	1:A:261:THR:HG22	2.44	0.48
1:B:275:ALA:HB2	1:B:304:ILE:HG21	1.95	0.48
2:D:32:MET:HE2	2:E:19:PRO:HB3	1.93	0.48
1:C:115:ILE:HD12	1:C:145:TYR:CZ	2.50	0.47
1:C:138:LEU:HD13	1:C:180:GLU:HB3	1.95	0.47
1:A:140:ASN:O	1:A:144:VAL:HG23	2.14	0.47
1:B:28:CYS:C	1:B:30:SER:H	2.18	0.47
1:C:152:PHE:HB2	1:C:167:VAL:HG22	1.96	0.47
1:C:178:TYR:CZ	1:C:200:ASN:HB3	2.49	0.47
1:B:20:LEU:HD21	1:B:46:VAL:HG21	1.97	0.47
1:A:311:ARG:NH2	1:A:344:ILE:HD13	2.29	0.46
1:B:20:LEU:HD11	1:B:43:ALA:N	2.30	0.46
1:B:37:VAL:O	1:B:41:GLU:HG2	2.16	0.46
1:B:54:LEU:HD11	1:B:58:TYR:OH	2.14	0.46
1:A:105:LEU:HD13	1:A:113:GLU:HB3	1.98	0.46
1:A:358:ARG:HH11	1:A:358:ARG:CA	2.29	0.46
1:B:111:PHE:O	1:B:115:ILE:HG13	2.15	0.46
1:C:186:THR:HG22	1:C:194:GLN:HG2	1.96	0.46
1:C:130:ASP:OD2	1:C:132:VAL:HG22	2.16	0.46
1:C:238:TYR:HB3	1:C:261:THR:HG23	1.98	0.46
1:C:352:SER:O	1:C:356:THR:HG23	2.16	0.46
2:E:62:LEU:C	2:E:62:LEU:HD13	2.35	0.46
1:B:185:VAL:HG11	1:B:193:ALA:HB3	1.98	0.45
1:B:231:LYS:HB3	1:B:268:LEU:HD21	1.98	0.45
1:C:29:LYS:NZ	2:F:60:GLY:H	2.15	0.45
1:B:318:CYS:SG	1:B:340:LYS:HB3	2.57	0.45
1:A:175:VAL:O	1:A:179:GLU:HG3	2.16	0.45
1:B:51:LEU:HA	1:B:54:LEU:HB3	1.98	0.45
1:C:23:GLU:HG2	1:C:39:PHE:CD2	2.51	0.45
2:D:47:LEU:HB2	2:D:63:ILE:HB	1.99	0.45
1:A:45:GLN:NE2	1:A:45:GLN:HA	2.31	0.45
1:B:23:GLU:O	1:B:27:LEU:HB2	2.16	0.45
1:B:68:LEU:O	1:B:69:HIS:HB2	2.17	0.45
1:A:238:TYR:CB	1:A:261:THR:CG2	2.95	0.45
1:A:344:ILE:O	1:A:348:VAL:HG22	2.17	0.45
1:B:75:LEU:HD12	1:B:101:LEU:CD1	2.46	0.45
1:A:226:LYS:NZ	1:A:238:TYR:OH	2.50	0.45
1:C:271:ARG:NH1	1:C:304:ILE:HG12	2.31	0.44
1:C:264:LEU:O	1:C:268:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:SER:HB2	2:E:50:LYS:HD2	2.00	0.44
1:C:221:ARG:NH2	1:C:233:ALA:CB	2.80	0.44
1:B:146:HIS:HD2	1:B:204:THR:OG1	2.01	0.44
1:C:16:SER:O	1:C:20:LEU:HG	2.16	0.44
1:A:136:ARG:NH1	2:D:48:GLN:HE21	2.11	0.43
2:D:67:GLY:O	2:D:68:PRO:C	2.56	0.43
1:A:40:PHE:HB3	1:A:61:LEU:HG	1.99	0.43
1:A:210:ASN:HA	1:B:210:ASN:HA	2.01	0.43
1:B:91:GLN:C	1:B:93:GLY:N	2.70	0.43
1:C:33:CYS:O	1:C:37:VAL:HG23	2.19	0.43
1:A:16:SER:OG	1:A:19:GLU:HG3	2.17	0.43
1:A:185:VAL:HG12	1:A:194:GLN:CG	2.43	0.43
1:C:164:PRO:HB2	1:C:167:VAL:HG23	2.01	0.43
1:A:325:TYR:CZ	1:A:333:GLN:HG2	2.54	0.43
1:A:37:VAL:O	1:A:41:GLU:HG2	2.18	0.42
1:A:223:LEU:HD13	3:A:442:HOH:O	2.18	0.42
1:B:296:ASP:O	1:B:300:LYS:HG3	2.19	0.42
1:C:270:ASP:CG	1:C:273:VAL:HG23	2.39	0.42
1:A:21:ALA:HB1	2:D:52:ILE:HD13	2.00	0.42
1:B:98:SER:HB3	1:B:117:CYS:O	2.18	0.42
2:E:24:GLN:HA	2:E:24:GLN:OE1	2.18	0.42
1:B:238:TYR:HB3	1:B:261:THR:HG22	1.98	0.42
1:B:52:LYS:HA	1:B:52:LYS:CE	2.47	0.42
1:B:88:ILE:HG13	1:B:90:ASP:HB2	2.01	0.42
1:C:115:ILE:HD12	1:C:145:TYR:CE1	2.54	0.42
1:A:146:HIS:CE1	1:A:150:LYS:HD2	2.55	0.42
1:B:60:GLN:NE2	2:E:52:ILE:HG13	2.35	0.42
1:A:339:GLU:HG3	1:A:361:LEU:HD21	2.01	0.42
1:B:78:HIS:CE1	1:B:100:ASN:HB3	2.55	0.42
1:C:338:ALA:O	1:C:341:HIS:HB3	2.20	0.41
1:A:129:ASN:HB2	3:A:434:HOH:O	2.21	0.41
1:B:91:GLN:C	1:B:93:GLY:H	2.22	0.41
1:B:267:GLN:C	1:B:269:LYS:H	2.22	0.41
1:C:117:CYS:O	1:C:120:ARG:HB3	2.20	0.41
2:F:62:LEU:HD21	2:F:64:LEU:HD21	2.03	0.41
1:A:258:TYR:HB3	1:A:281:LEU:HG	2.02	0.41
1:B:311:ARG:HA	1:B:311:ARG:HD2	1.83	0.41
1:C:319:TRP:HB2	1:C:341:HIS:CE1	2.55	0.41
1:B:325:TYR:CZ	1:B:333:GLN:HG2	2.56	0.41
1:A:63:ASN:ND2	1:A:78:HIS:HE1	2.18	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	351/406 (86%)	347 (99%)	4 (1%)	0	100	100
1	B	346/406 (85%)	331 (96%)	14 (4%)	1 (0%)	41	64
1	C	342/406 (84%)	335 (98%)	7 (2%)	0	100	100
2	D	43/52 (83%)	40 (93%)	3 (7%)	0	100	100
2	E	37/52 (71%)	33 (89%)	4 (11%)	0	100	100
2	F	44/52 (85%)	36 (82%)	8 (18%)	0	100	100
All	All	1163/1374 (85%)	1122 (96%)	40 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	LEU

### 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	278/327 (85%)	275 (99%)	3 (1%)	73	88
1	B	266/327 (81%)	259 (97%)	7 (3%)	46	72
1	C	269/327 (82%)	267 (99%)	2 (1%)	84	94
2	D	39/43 (91%)	39 (100%)	0	100	100
2	E	33/43 (77%)	33 (100%)	0	100	100
2	F	37/43 (86%)	36 (97%)	1 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	922/1110 (83%)	909 (99%)	13 (1%)	67 85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	A	223	LEU
1	A	358	ARG
1	B	79	HIS
1	B	121	HIS
1	B	221	ARG
1	B	223	LEU
1	B	309	ASN
1	B	332	ASP
1	B	356	THR
1	C	266	ARG
1	C	332	ASP
2	F	57	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	63	ASN
1	A	78	HIS
1	A	146	HIS
1	A	331	HIS
1	B	60	GLN
1	B	63	ASN
1	B	103	ASN
1	B	119	GLN
1	B	129	ASN
1	B	146	HIS
1	B	181	ASN
1	B	267	GLN
1	B	309	ASN
1	B	333	GLN
1	B	360	ASN
1	C	45	GLN
1	C	63	ASN
1	C	121	HIS

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Mol	Chain	Res	Type
1	C	146	HIS
1	C	267	GLN
1	C	330	ASN
1	C	333	GLN
1	C	341	HIS
2	D	48	GLN
2	E	48	GLN
2	F	48	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 monosaccharides 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, 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	355/406 (87%)	-0.16	4 (1%) 80 78	20, 38, 60, 79	0
1	B	350/406 (86%)	0.19	30 (8%) 10 7	22, 46, 121, 129	0
1	C	346/406 (85%)	-0.08	3 (0%) 84 82	21, 40, 77, 99	0
2	D	45/52 (86%)	0.71	8 (17%) 1 0	28, 45, 99, 103	0
2	E	41/52 (78%)	0.55	4 (9%) 7 5	9, 58, 93, 99	1 (2%)
2	F	46/52 (88%)	0.75	10 (21%) 0 0	33, 53, 104, 110	0
All	All	1183/1374 (86%)	0.06	59 (4%) 28 23	9, 42, 99, 129	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	57	ASP	5.2
1	B	44	VAL	5.0
2	D	56	GLU	4.9
1	B	89	GLY	4.8
2	F	56	GLU	4.4
2	D	67	GLY	4.3
2	D	68	PRO	4.2
1	A	13	MET	4.2
1	B	88	ILE	4.1
2	D	54	LEU	4.0
1	B	92	LEU	4.0
2	D	59	GLN	4.0
2	F	58	ALA	3.9
2	F	68	PRO	3.9
1	B	90	ASP	3.7
2	D	57	ASP	3.6
1	B	348	VAL	3.5
1	A	15	ALA	3.4
2	F	23	MET	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	58	ALA	3.2
1	B	58	TYR	3.1
1	B	67	TYR	3.0
1	B	46	VAL	3.0
2	F	59	GLN	3.0
1	B	77	TYR	3.0
2	D	60	GLY	3.0
1	B	52	LYS	3.0
2	E	23	MET	2.9
1	B	153	GLY	2.9
2	F	54	LEU	2.9
1	B	51	LEU	2.8
1	B	84	LEU	2.7
1	B	85	ALA	2.7
2	F	60	GLY	2.7
1	B	33	CYS	2.5
1	B	50	ASP	2.5
1	B	47	GLY	2.5
2	E	49	ALA	2.5
1	B	49	GLU	2.4
2	F	67	GLY	2.4
1	B	57	ILE	2.4
1	B	32	ASP	2.4
1	B	95	ALA	2.4
1	B	56	ALA	2.4
1	B	68	LEU	2.3
1	A	153	GLY	2.3
1	B	53	THR	2.3
2	E	31	TRP	2.3
1	C	365	GLN	2.3
1	C	15	ALA	2.2
1	B	91	GLN	2.2
2	E	21	GLY	2.1
1	B	21	ALA	2.1
1	B	66	PHE	2.1
1	C	21	ALA	2.1
1	A	374	THR	2.1
1	B	160	VAL	2.0
2	F	24	GLN	2.0
1	B	128	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.