



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3T06  
Title : Crystal Structure of the DH/PH fragment of PDZRHOGEF with N-terminal regulatory elements in complex with Human RhoA  
Authors : Bielnicki, J.A.; Derewenda, U.; Derewenda, Z.S.  
Deposited on : 2011-07-19  
Resolution : 2.84 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  
<http://wwpdb.org/validation/2016/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  
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

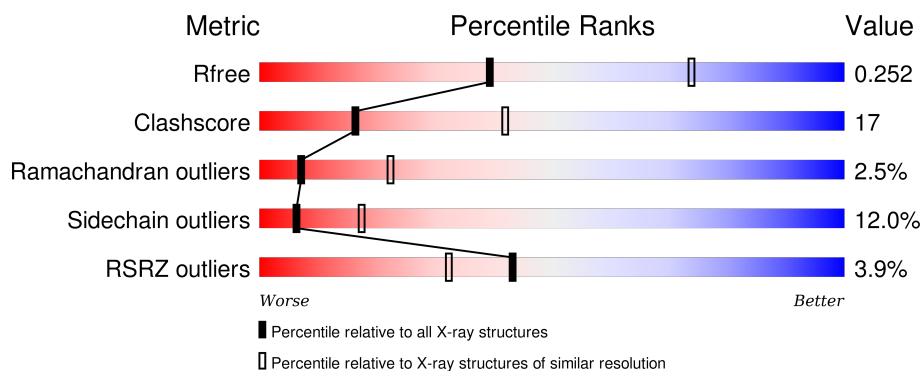
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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. 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	418	<div> <div>3%</div> <div>52% 26% 6% 15%</div> </div>
1	E	418	<div> <div>4%</div> <div>54% 24% 8% 14%</div> </div>
2	B	178	<div> <div>3%</div> <div>59% 39% .</div> </div>
2	F	178	<div> <div>3%</div> <div>62% 34% .</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8657 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 Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2905	1837	519	534	15			
1	E	358	Total	C	N	O	S	0	0	0
			2930	1852	525	538	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1082	HIS	-	EXPRESSION TAG	UNP O15085
A	1083	HIS	-	EXPRESSION TAG	UNP O15085
A	1084	HIS	-	EXPRESSION TAG	UNP O15085
A	1085	HIS	-	EXPRESSION TAG	UNP O15085
A	1086	HIS	-	EXPRESSION TAG	UNP O15085
A	1087	HIS	-	EXPRESSION TAG	UNP O15085
A	1088	HIS	-	EXPRESSION TAG	UNP O15085
A	1089	HIS	-	EXPRESSION TAG	UNP O15085
E	1082	HIS	-	EXPRESSION TAG	UNP O15085
E	1083	HIS	-	EXPRESSION TAG	UNP O15085
E	1084	HIS	-	EXPRESSION TAG	UNP O15085
E	1085	HIS	-	EXPRESSION TAG	UNP O15085
E	1086	HIS	-	EXPRESSION TAG	UNP O15085
E	1087	HIS	-	EXPRESSION TAG	UNP O15085
E	1088	HIS	-	EXPRESSION TAG	UNP O15085
E	1089	HIS	-	EXPRESSION TAG	UNP O15085

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			
2	F	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			

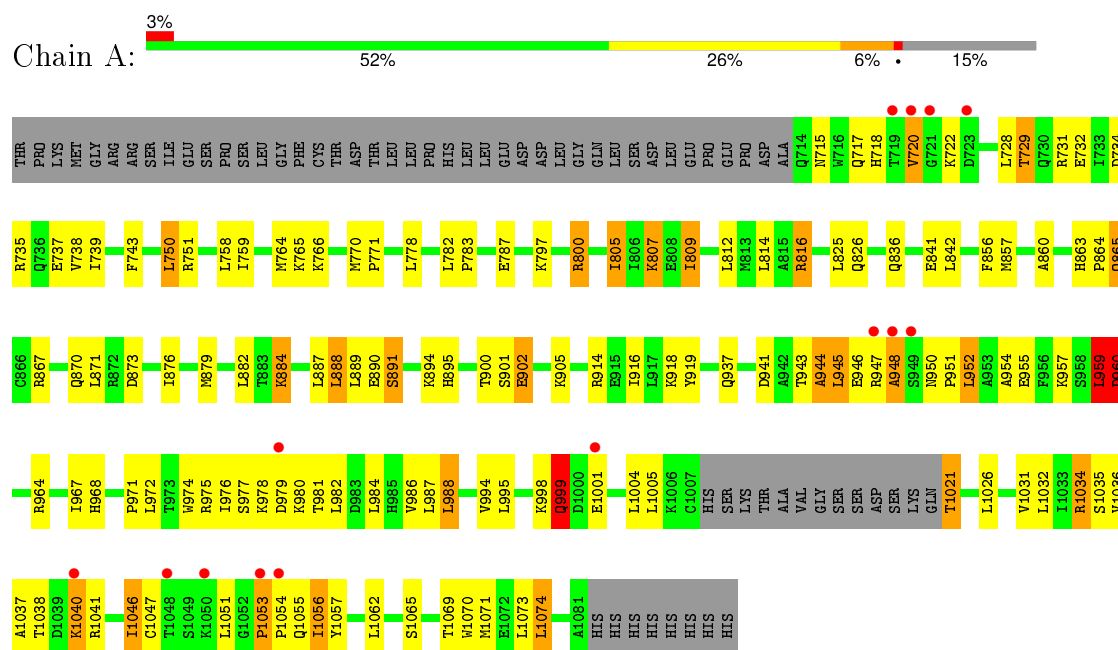
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	ENGINEERED MUTATION	UNP P61586
F	25	ASN	PHE	ENGINEERED MUTATION	UNP P61586

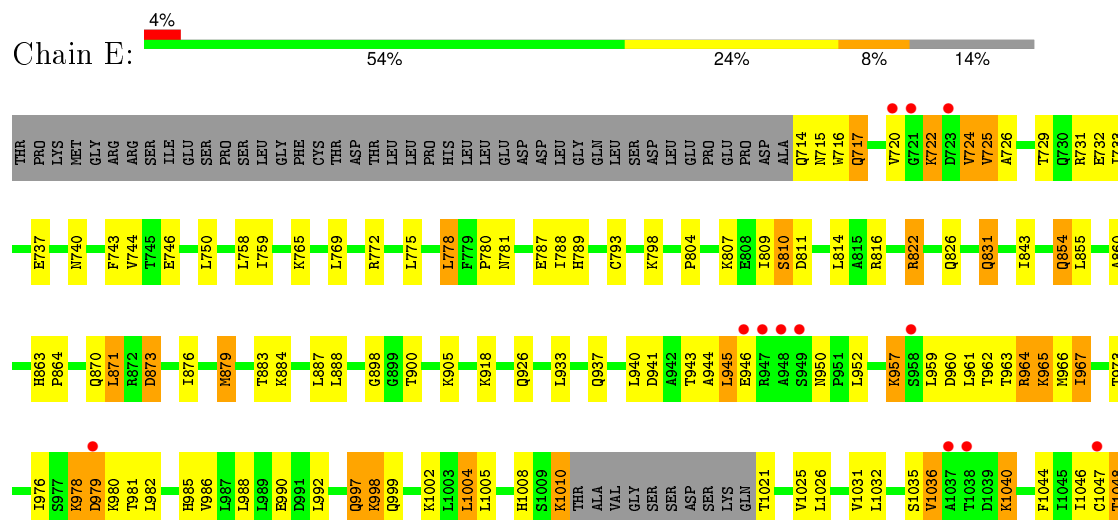
### 3 Residue-property plots

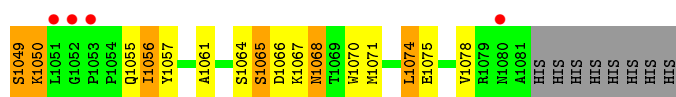
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Rho guanine nucleotide exchange factor 11



- Molecule 1: Rho guanine nucleotide exchange factor 11





• Molecule 2: Transforming protein RhoA



• Molecule 2: Transforming protein RhoA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.37Å 118.63Å 92.44Å 90.00° 113.61° 90.00°	Depositor
Resolution (Å)	29.82 – 2.84 29.82 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.82-2.84) 93.6 (29.82-2.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_818)	Depositor
R, $R_{free}$	0.208 , 0.257 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	1849 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 36883 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/2949	0.62	0/3970
1	E	0.50	0/2975	0.64	0/4004
2	B	0.51	0/1438	0.63	0/1944
2	F	0.51	0/1438	0.65	0/1944
All	All	0.50	0/8800	0.63	0/11862

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	2905	0	2997	102	0
1	E	2930	0	3022	97	0
2	B	1411	0	1402	52	0
2	F	1411	0	1402	47	0
All	All	8657	0	8823	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (292) 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:900:THR:HG22	1:A:902:GLU:H	1.33	0.91
1:E:1056:ILE:H	1:E:1056:ILE:HD12	1.39	0.87
1:A:1053:PRO:HB3	1:A:1054:PRO:HD2	1.58	0.86
2:F:18:LYS:NZ	2:F:64:GLU:OE2	2.10	0.85
2:F:30:PHE:CD1	2:F:31:PRO:HD2	2.13	0.84
1:A:947:ARG:HG3	1:A:948:ALA:H	1.43	0.82
1:E:941:ASP:HB3	1:E:1004:LEU:HB3	1.64	0.80
1:A:1046:ILE:HG23	1:A:1056:ILE:HG13	1.64	0.78
1:A:1034:ARG:HH11	1:A:1035:SER:H	1.28	0.78
1:A:825:LEU:HD23	1:A:916:ILE:HD13	1.67	0.77
1:A:884:LYS:HG3	2:B:38:VAL:HG22	1.70	0.74
2:F:122:ARG:NH2	2:F:158:GLU:OE1	2.22	0.73
2:B:85:SER:OG	2:B:118:LYS:HD2	1.89	0.73
1:A:943:THR:O	1:A:945:LEU:N	2.21	0.73
2:B:16:CYS:HB2	2:B:85:SER:HB2	1.71	0.72
1:A:900:THR:HG22	1:A:902:GLU:N	2.05	0.72
2:F:16:CYS:HB2	2:F:85:SER:HB2	1.71	0.71
1:E:976:ILE:HD12	1:E:980:LYS:HE3	1.72	0.71
1:E:950:ASN:ND2	1:E:1021:THR:O	2.24	0.71
1:E:898:GLY:O	1:E:900:THR:HG23	1.91	0.70
2:F:117:ASN:OD1	2:F:118:LYS:N	2.24	0.70
1:E:1005:LEU:HD12	1:E:1005:LEU:O	1.91	0.70
1:A:717:GLN:HG3	1:A:737:GLU:OE2	1.91	0.70
1:E:1026:LEU:HD21	1:E:1057:TYR:CE1	2.27	0.70
2:B:157:MET:HG2	2:B:170:VAL:HG22	1.72	0.69
2:F:21:LEU:HD22	2:F:171:PHE:HE2	1.57	0.69
1:E:1036:VAL:HG22	1:E:1044:PHE:CE2	2.28	0.69
1:E:1056:ILE:N	1:E:1056:ILE:HD12	2.07	0.69
1:A:816:ARG:HD3	1:A:816:ARG:O	1.91	0.68
1:A:1026:LEU:HD21	1:A:1057:TYR:CE1	2.29	0.67
1:E:816:ARG:HD3	1:E:816:ARG:O	1.94	0.67
2:F:6:LYS:HD2	2:F:178:ALA:HB1	1.76	0.67
1:A:879:MET:HE2	2:B:69:LEU:HB3	1.76	0.67
2:B:24:VAL:HG12	2:B:30:PHE:HA	1.77	0.67
2:F:19:THR:O	2:F:23:ILE:HG12	1.95	0.67
1:E:926:GLN:HA	1:E:926:GLN:OE1	1.95	0.67
1:A:715:ASN:HD22	1:A:718:HIS:CD2	2.13	0.66
2:F:85:SER:OG	2:F:118:LYS:HD3	1.95	0.66
2:B:100:THR:N	2:B:101:PRO:HD2	2.10	0.66
1:A:826:GLN:HB2	1:A:919:TYR:CD1	2.30	0.66
1:E:941:ASP:HB2	1:E:1002:LYS:HE2	1.78	0.66
1:E:1048:THR:O	1:E:1050:LYS:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:LEU:HD22	1:A:1005:LEU:HB3	1.78	0.66
1:A:738:VAL:HG11	1:A:891:SER:HB3	1.79	0.64
1:E:1048:THR:O	1:E:1050:LYS:N	2.30	0.64
1:E:717:GLN:HG2	1:E:737:GLU:OE2	1.98	0.64
1:A:870:GLN:HG3	2:B:5:ARG:HH12	1.62	0.63
1:E:943:THR:C	1:E:945:LEU:H	2.01	0.63
1:E:765:LYS:O	1:E:772:ARG:NH2	2.31	0.63
2:F:4:ILE:O	2:F:4:ILE:HG13	1.98	0.63
2:F:162:LYS:H	2:F:162:LYS:HD2	1.63	0.63
2:F:81:LEU:HD23	2:F:113:ILE:HG12	1.81	0.63
1:E:964:ARG:HD3	1:E:992:LEU:HD12	1.82	0.62
1:E:1064:SER:O	1:E:1068:ASN:OD1	2.18	0.61
1:A:728:LEU:HD22	1:A:732:GLU:HG2	1.82	0.61
1:A:1053:PRO:HB3	1:A:1054:PRO:CD	2.30	0.61
1:A:1034:ARG:HH11	1:A:1035:SER:N	1.97	0.61
2:B:119:LYS:C	2:B:121:LEU:H	2.04	0.61
1:E:978:LYS:O	1:E:979:ASP:HB2	2.00	0.61
2:F:80:ILE:HD13	2:F:103:VAL:HG13	1.82	0.61
2:B:24:VAL:HG23	2:B:25:ASN:H	1.66	0.60
1:E:937:GLN:HA	1:E:937:GLN:OE1	2.01	0.60
2:B:95:ILE:O	2:B:100:THR:HG23	2.02	0.60
1:E:1031:VAL:HG12	1:E:1047:CYS:HA	1.84	0.60
1:A:1040:LYS:H	1:A:1040:LYS:HD3	1.68	0.59
2:F:175:THR:O	2:F:179:LEU:HG	2.02	0.59
2:B:166:GLY:O	2:B:170:VAL:HG23	2.03	0.59
1:E:810:SER:HB2	1:E:905:LYS:HB3	1.83	0.59
1:A:977:SER:HB2	1:A:980:LYS:HB3	1.83	0.59
1:A:943:THR:C	1:A:945:LEU:H	2.05	0.58
1:A:1040:LYS:HE2	1:A:1041:ARG:NH1	2.17	0.58
2:B:17:GLY:HA3	2:B:117:ASN:HD22	1.68	0.58
1:A:1026:LEU:HD21	1:A:1057:TYR:CZ	2.38	0.58
1:A:967:ILE:HD12	1:A:988:LEU:HD13	1.85	0.58
1:A:914:ARG:O	1:A:918:LYS:HG3	2.04	0.58
1:E:740:ASN:O	1:E:744:VAL:HG23	2.03	0.58
2:B:19:THR:O	2:B:23:ILE:HG13	2.04	0.58
1:A:1053:PRO:CB	1:A:1054:PRO:HD2	2.31	0.58
1:E:778:LEU:O	1:E:780:PRO:HD3	2.04	0.57
1:E:781:ASN:HD21	1:E:831:GLN:HB3	1.69	0.57
1:E:997:GLN:HB3	1:E:1004:LEU:HD12	1.86	0.57
1:E:1040:LYS:O	1:E:1067:LYS:HD3	2.04	0.57
1:A:729:THR:HG23	1:A:732:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1008:HIS:O	1:E:1021:THR:HB	2.04	0.57
2:B:113:ILE:O	2:B:113:ILE:HG13	2.04	0.56
2:B:10:ILE:HD11	2:B:83:CYS:SG	2.45	0.56
1:E:814:LEU:HD11	1:E:905:LYS:HG2	1.86	0.56
1:A:1053:PRO:CB	1:A:1054:PRO:CD	2.84	0.56
2:F:162:LYS:N	2:F:162:LYS:HD2	2.21	0.55
1:E:985:HIS:HB2	1:E:998:LYS:HE3	1.86	0.55
2:B:82:MET:SD	2:B:100:THR:HG22	2.47	0.55
1:E:854:GLN:O	1:E:854:GLN:HG2	2.05	0.55
1:A:1034:ARG:NH1	1:A:1035:SER:H	2.00	0.55
2:B:125:GLU:OE1	2:B:129:ARG:NH1	2.40	0.55
1:E:1065:SER:HA	1:E:1068:ASN:OD1	2.07	0.55
1:A:814:LEU:HD11	1:A:905:LYS:HG2	1.88	0.55
2:B:10:ILE:O	2:B:10:ILE:HG23	2.05	0.55
2:F:140:LYS:HB3	2:F:142:GLU:OE1	2.06	0.55
2:B:122:ARG:NH1	2:B:139:VAL:O	2.37	0.55
1:E:976:ILE:HD11	1:E:982:LEU:HG	1.88	0.54
1:A:1065:SER:O	1:A:1069:THR:HG23	2.08	0.54
1:A:947:ARG:O	1:A:948:ALA:HB3	2.08	0.54
1:E:965:LYS:HG2	1:E:990:GLU:HG3	1.90	0.54
1:A:1036:VAL:HG12	1:A:1037:ALA:N	2.23	0.54
1:E:1049:SER:O	1:E:1050:LYS:O	2.25	0.54
1:A:1034:ARG:NH1	1:A:1035:SER:HB3	2.23	0.54
2:F:86:ILE:O	2:F:139:VAL:HG23	2.08	0.54
1:E:876:ILE:O	1:E:876:ILE:HG12	2.07	0.54
2:B:6:LYS:HD2	2:B:178:ALA:HB1	1.89	0.54
2:F:21:LEU:HD22	2:F:171:PHE:CE2	2.41	0.54
1:E:720:VAL:HG12	1:E:804:PRO:HB3	1.90	0.54
2:B:157:MET:CG	2:B:170:VAL:HG22	2.39	0.54
1:E:759:ILE:HG22	1:E:860:ALA:HB1	1.90	0.54
1:A:941:ASP:HB3	1:A:1004:LEU:HD23	1.90	0.53
1:A:743:PHE:HB3	1:A:800:ARG:HH21	1.73	0.53
2:B:63:GLN:O	2:B:70:ARG:HG3	2.08	0.53
1:A:1046:ILE:HG12	1:A:1056:ILE:HD11	1.89	0.53
1:E:863:HIS:ND1	1:E:864:PRO:HD2	2.23	0.53
1:A:766:LYS:HG3	1:A:766:LYS:O	2.07	0.53
1:A:1040:LYS:HE2	1:A:1041:ARG:HH12	1.74	0.52
1:E:959:LEU:HD22	1:E:961:LEU:HD23	1.92	0.52
1:E:822:ARG:HD2	1:E:826:GLN:OE1	2.09	0.52
1:A:975:ARG:HG3	1:A:981:THR:HG22	1.89	0.52
1:A:728:LEU:HD11	1:A:805:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:778:LEU:C	1:E:780:PRO:HD3	2.30	0.52
2:F:17:GLY:HA3	2:F:117:ASN:ND2	2.25	0.52
2:B:24:VAL:HG23	2:B:25:ASN:N	2.25	0.52
1:E:946:GLU:HG2	1:E:957:LYS:HB2	1.91	0.52
1:E:933:LEU:HD11	1:E:966:MET:HB2	1.92	0.51
1:A:950:ASN:ND2	1:A:952:LEU:HB2	2.25	0.51
1:A:978:LYS:O	1:A:980:LYS:N	2.44	0.51
2:F:122:ARG:HH22	2:F:158:GLU:CD	2.14	0.51
1:E:967:ILE:N	1:E:967:ILE:HD13	2.25	0.51
1:A:863:HIS:HD2	1:A:865:GLN:H	1.57	0.51
2:B:157:MET:HG2	2:B:170:VAL:CG2	2.38	0.51
1:A:1046:ILE:HG23	1:A:1056:ILE:CG1	2.36	0.51
2:F:81:LEU:CD2	2:F:113:ILE:HG12	2.40	0.51
1:A:1036:VAL:HG12	1:A:1037:ALA:H	1.75	0.51
1:E:1026:LEU:HD21	1:E:1057:TYR:CD1	2.45	0.50
1:A:937:GLN:OE1	1:A:960:ASP:HA	2.11	0.50
1:A:945:LEU:HD13	1:A:1005:LEU:O	2.11	0.50
1:A:976:ILE:HG23	1:A:980:LYS:HD3	1.93	0.50
2:B:10:ILE:HG21	2:B:22:LEU:HD11	1.92	0.50
2:F:82:MET:HG2	2:F:95:ILE:HD12	1.94	0.50
1:E:733:ILE:O	1:E:737:GLU:HG2	2.12	0.50
2:F:80:ILE:HD13	2:F:103:VAL:CG1	2.42	0.50
1:E:787:GLU:OE1	1:E:787:GLU:HA	2.12	0.50
1:A:856:PHE:HD1	1:A:857:MET:HE2	1.77	0.49
1:A:1031:VAL:HA	1:A:1046:ILE:O	2.12	0.49
1:A:739:ILE:HG12	1:A:809:ILE:HD12	1.95	0.49
1:E:937:GLN:NE2	1:E:960:ASP:HA	2.28	0.49
1:A:968:HIS:HB2	1:A:1073:LEU:HD13	1.94	0.49
2:B:110:VAL:HG13	2:B:111:PRO:HD2	1.94	0.49
1:E:863:HIS:CG	1:E:864:PRO:HD2	2.48	0.49
1:A:873:ASP:O	1:A:876:ILE:HG22	2.13	0.49
1:E:716:TRP:HB3	1:E:737:GLU:OE1	2.13	0.48
2:F:22:LEU:HD23	2:F:171:PHE:HZ	1.78	0.48
1:E:1040:LYS:HB2	1:E:1064:SER:HB3	1.95	0.48
2:B:70:ARG:HH11	2:B:70:ARG:HG3	1.78	0.48
1:A:987:LEU:HB2	1:A:994:VAL:HG22	1.93	0.48
1:A:984:LEU:HD13	1:A:995:LEU:HD22	1.95	0.48
1:E:1061:ALA:HB1	1:E:1066:ASP:HB3	1.96	0.48
1:A:759:ILE:HG22	1:A:860:ALA:HB1	1.96	0.48
1:E:788:ILE:HG22	1:E:789:HIS:N	2.28	0.48
1:E:1070:TRP:O	1:E:1074:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:999:GLN:HB3	1:E:1002:LYS:HB3	1.94	0.48
1:E:1068:ASN:N	1:E:1068:ASN:OD1	2.36	0.48
1:A:1040:LYS:N	1:A:1040:LYS:HD3	2.29	0.48
2:B:163:THR:O	2:B:164:LYS:HB2	2.14	0.48
1:E:978:LYS:HD2	1:E:979:ASP:H	1.78	0.47
1:A:863:HIS:CD2	1:A:864:PRO:HD2	2.49	0.47
1:A:1021:THR:O	1:A:1055:GLN:NE2	2.47	0.47
1:A:1056:ILE:O	1:A:1056:ILE:HG22	2.14	0.47
1:E:1035:SER:HG	1:E:1067:LYS:HZ1	1.54	0.47
1:E:722:LYS:O	1:E:725:VAL:HG12	2.14	0.47
1:E:943:THR:O	1:E:945:LEU:N	2.46	0.47
2:B:81:LEU:HD23	2:B:113:ILE:CG1	2.45	0.47
2:F:68:ARG:HA	2:F:68:ARG:HD2	1.64	0.47
1:E:964:ARG:CD	1:E:992:LEU:HD12	2.45	0.47
2:B:122:ARG:HH22	2:B:158:GLU:CD	2.18	0.47
1:A:1034:ARG:HH12	1:A:1035:SER:HB3	1.80	0.47
1:A:974:TRP:CZ2	1:A:1057:TYR:CD2	3.03	0.47
1:E:724:VAL:C	1:E:726:ALA:H	2.16	0.47
2:B:17:GLY:O	2:B:18:LYS:C	2.52	0.47
1:E:918:LYS:HB3	1:E:918:LYS:HE2	1.66	0.47
1:A:888:LEU:HD12	1:A:888:LEU:HA	1.73	0.47
1:E:717:GLN:CG	1:E:737:GLU:OE2	2.62	0.46
1:A:976:ILE:CG2	1:A:980:LYS:HD3	2.45	0.46
2:B:23:ILE:HD13	2:B:36:PRO:HD2	1.97	0.46
1:A:951:PRO:HA	1:A:954:ALA:HB2	1.97	0.46
1:E:943:THR:C	1:E:945:LEU:N	2.68	0.46
1:A:950:ASN:HD22	1:A:952:LEU:HD13	1.79	0.46
1:A:1070:TRP:O	1:A:1074:LEU:HB2	2.15	0.46
1:E:871:LEU:HD22	1:E:871:LEU:O	2.15	0.46
1:E:870:GLN:HG3	2:F:5:ARG:HH12	1.80	0.46
2:F:120:ASP:OD1	2:F:160:SER:HB2	2.15	0.46
1:E:729:THR:HG23	1:E:732:GLU:H	1.81	0.46
2:F:95:ILE:HB	2:F:96:PRO:HD3	1.97	0.46
2:F:100:THR:N	2:F:101:PRO:HD2	2.30	0.46
1:E:952:LEU:H	1:E:952:LEU:HD12	1.81	0.46
1:A:750:LEU:HD23	1:A:750:LEU:HA	1.74	0.46
2:B:48:VAL:HG23	2:B:48:VAL:O	2.15	0.46
1:A:943:THR:C	1:A:945:LEU:N	2.69	0.45
2:F:110:VAL:HG13	2:F:111:PRO:HD2	1.98	0.45
1:A:876:ILE:O	1:A:876:ILE:HG12	2.16	0.45
2:B:7:LYS:HE3	2:B:58:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:PRO:O	2:F:109:ASN:HB2	2.16	0.45
1:E:1036:VAL:HG13	1:E:1044:PHE:HE2	1.81	0.45
2:B:119:LYS:O	2:B:121:LEU:N	2.48	0.45
1:E:960:ASP:OD1	1:E:963:THR:HG23	2.17	0.45
1:A:1040:LYS:H	1:A:1040:LYS:CD	2.24	0.45
1:A:959:LEU:O	1:A:960:ASP:HB2	2.17	0.45
1:E:781:ASN:ND2	1:E:831:GLN:HB3	2.30	0.45
1:E:879:MET:O	1:E:883:THR:HG23	2.17	0.45
2:B:9:VAL:HG22	2:B:58:TRP:HB2	1.99	0.45
1:A:770:MET:HB2	1:A:771:PRO:HD2	1.99	0.45
1:A:734:ASP:O	1:A:738:VAL:HG23	2.17	0.45
1:A:937:GLN:HG3	1:A:937:GLN:O	2.17	0.45
1:E:1031:VAL:O	1:E:1032:LEU:HD13	2.17	0.44
1:A:971:PRO:O	1:A:972:LEU:HD13	2.17	0.44
1:E:1046:ILE:HG13	1:E:1056:ILE:HG23	1.98	0.44
2:B:74:TYR:N	2:B:75:PRO:CD	2.80	0.44
1:A:1032:LEU:HA	1:A:1032:LEU:HD23	1.85	0.44
2:F:10:ILE:O	2:F:10:ILE:HG23	2.16	0.44
1:E:1075:GLU:O	1:E:1078:VAL:HG12	2.16	0.44
2:F:166:GLY:O	2:F:170:VAL:HG23	2.17	0.44
1:A:999:GLN:HG2	1:A:1004:LEU:CD1	2.48	0.44
2:F:157:MET:HB3	2:F:170:VAL:HG22	1.99	0.44
1:A:1005:LEU:HA	1:A:1005:LEU:HD23	1.82	0.44
1:E:715:ASN:OD1	2:F:33:VAL:HG11	2.17	0.44
1:A:977:SER:HB2	1:A:980:LYS:HD2	1.99	0.44
1:A:943:THR:HG22	1:A:944:ALA:N	2.32	0.44
2:B:100:THR:N	2:B:101:PRO:CD	2.80	0.44
1:A:751:ARG:HH22	1:A:867:ARG:HD3	1.83	0.44
1:A:890:GLU:OE1	1:A:914:ARG:NH2	2.50	0.44
2:F:75:PRO:O	2:F:76:ASP:HB2	2.17	0.43
2:F:122:ARG:NH1	2:F:139:VAL:O	2.40	0.43
2:F:154:PHE:CD2	2:F:177:ALA:HB2	2.52	0.43
2:B:103:VAL:O	2:B:107:CYS:HB2	2.17	0.43
1:E:1065:SER:HB3	2:F:97:GLU:HG3	1.99	0.43
1:E:879:MET:SD	1:E:879:MET:C	2.96	0.43
2:F:17:GLY:O	2:F:18:LYS:C	2.56	0.43
2:B:77:THR:HG22	2:B:110:VAL:HG11	1.99	0.43
1:A:1035:SER:HB2	1:A:1071:MET:CE	2.49	0.43
1:A:737:GLU:OE1	1:A:737:GLU:HA	2.18	0.43
1:E:1067:LYS:HG2	1:E:1068:ASN:N	2.33	0.43
2:B:70:ARG:N	2:B:71:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LYS:C	2:B:121:LEU:N	2.71	0.43
2:F:110:VAL:CG1	2:F:111:PRO:HD2	2.48	0.43
2:F:157:MET:CB	2:F:170:VAL:HG22	2.48	0.43
1:E:1067:LYS:HE3	1:E:1071:MET:CE	2.49	0.43
1:E:978:LYS:HD2	1:E:979:ASP:N	2.32	0.43
1:E:724:VAL:O	1:E:726:ALA:N	2.52	0.43
2:B:24:VAL:O	2:B:25:ASN:C	2.55	0.42
1:A:782:LEU:HB3	1:A:783:PRO:HD3	1.99	0.42
1:E:743:PHE:O	1:E:746:GLU:HB3	2.20	0.42
2:B:17:GLY:HA3	2:B:117:ASN:ND2	2.31	0.42
2:F:70:ARG:N	2:F:71:PRO:CD	2.81	0.42
1:A:946:GLU:CB	1:A:957:LYS:HD2	2.50	0.42
1:E:724:VAL:C	1:E:726:ALA:N	2.73	0.42
2:B:70:ARG:O	2:B:73:SER:HB2	2.20	0.42
2:F:95:ILE:HB	2:F:96:PRO:CD	2.50	0.42
1:E:1046:ILE:O	1:E:1046:ILE:HG22	2.20	0.42
2:F:21:LEU:CD2	2:F:167:VAL:HG13	2.50	0.42
1:E:775:LEU:HD12	1:E:775:LEU:HA	1.84	0.42
1:E:781:ASN:N	1:E:781:ASN:OD1	2.49	0.42
1:E:986:VAL:HG22	1:E:1070:TRP:CH2	2.55	0.42
1:A:787:GLU:HA	1:A:787:GLU:OE1	2.20	0.42
1:A:807:LYS:HB2	1:A:807:LYS:HE2	1.87	0.42
1:A:900:THR:HG21	1:A:902:GLU:HB3	2.02	0.41
1:E:992:LEU:HD22	1:E:1025:VAL:CG1	2.50	0.41
1:A:1073:LEU:HD23	1:A:1073:LEU:HA	1.78	0.41
2:B:179:LEU:O	2:B:180:GLN:C	2.58	0.41
2:B:142:GLU:CD	2:B:142:GLU:H	2.24	0.41
2:F:24:VAL:HG12	2:F:30:PHE:HA	2.02	0.41
1:A:735:ARG:HD2	1:A:895:HIS:O	2.20	0.41
2:B:174:ALA:O	2:B:177:ALA:HB3	2.20	0.41
1:A:728:LEU:HD11	1:A:805:ILE:HD13	2.03	0.41
1:E:1010:LYS:C	1:E:1010:LYS:HE2	2.41	0.41
1:E:781:ASN:ND2	1:E:831:GLN:OE1	2.54	0.41
2:B:129:ARG:O	2:B:132:ALA:HB3	2.20	0.41
1:A:959:LEU:O	1:A:960:ASP:CB	2.69	0.41
2:B:27:LYS:O	2:B:29:GLN:HG2	2.21	0.41
1:E:946:GLU:HA	1:E:957:LYS:HB3	2.04	0.40
1:E:809:ILE:O	1:E:811:ASP:N	2.54	0.40
1:E:873:ASP:N	1:E:873:ASP:OD1	2.54	0.40
2:B:95:ILE:HG22	2:B:96:PRO:N	2.37	0.40
1:A:999:GLN:HG2	1:A:1004:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:HA	1:A:889:LEU:HD23	1.94	0.40
2:F:87:ASP:C	2:F:87:ASP:OD1	2.60	0.40
1:A:764:MET:HE1	1:A:857:MET:HE3	2.04	0.40
1:A:946:GLU:HA	1:A:957:LYS:HD2	2.03	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	351/418 (84%)	310 (88%)	31 (9%)	10 (3%)	6	19
1	E	354/418 (85%)	316 (89%)	28 (8%)	10 (3%)	6	19
2	B	176/178 (99%)	159 (90%)	14 (8%)	3 (2%)	11	34
2	F	176/178 (99%)	158 (90%)	15 (8%)	3 (2%)	11	34
All	All	1057/1192 (89%)	943 (89%)	88 (8%)	26 (2%)	7	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	944	ALA
1	A	948	ALA
1	A	959	LEU
1	A	979	ASP
1	A	1053	PRO
2	B	120	ASP
1	E	1049	SER
1	E	1050	LYS
2	B	67	ASP
1	E	944	ALA
1	E	962	THR

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Mol	Chain	Res	Type
1	E	1048	THR
1	A	807	LYS
2	B	18	LYS
1	E	810	SER
1	E	1040	LYS
2	F	18	LYS
1	A	999	GLN
2	F	32	GLU
1	A	720	VAL
1	A	960	ASP
1	E	722	LYS
1	A	800	ARG
1	E	979	ASP
2	F	33	VAL
1	E	725	VAL

### 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	323/380 (85%)	275 (85%)	48 (15%)	4	10
1	E	326/380 (86%)	284 (87%)	42 (13%)	5	14
2	B	156/156 (100%)	144 (92%)	12 (8%)	16	40
2	F	156/156 (100%)	143 (92%)	13 (8%)	14	36
All	All	961/1072 (90%)	846 (88%)	115 (12%)	6	17

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	VAL
1	A	722	LYS
1	A	729	THR
1	A	731	ARG
1	A	750	LEU
1	A	758	LEU

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Mol	Chain	Res	Type
1	A	765	LYS
1	A	778	LEU
1	A	797	LYS
1	A	805	ILE
1	A	809	ILE
1	A	812	LEU
1	A	816	ARG
1	A	836	GLN
1	A	841	GLU
1	A	842	LEU
1	A	865	GLN
1	A	871	LEU
1	A	882	LEU
1	A	884	LYS
1	A	887	LEU
1	A	888	LEU
1	A	891	SER
1	A	894	LYS
1	A	901	SER
1	A	902	GLU
1	A	945	LEU
1	A	952	LEU
1	A	955	GLU
1	A	959	LEU
1	A	960	ASP
1	A	964	ARG
1	A	982	LEU
1	A	986	VAL
1	A	988	LEU
1	A	998	LYS
1	A	999	GLN
1	A	1001	GLU
1	A	1021	THR
1	A	1034	ARG
1	A	1038	THR
1	A	1040	LYS
1	A	1046	ILE
1	A	1047	CYS
1	A	1051	LEU
1	A	1056	ILE
1	A	1062	LEU
1	A	1074	LEU

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Mol	Chain	Res	Type
2	B	16	CYS
2	B	20	CYS
2	B	32	GLU
2	B	33	VAL
2	B	35	VAL
2	B	55	LEU
2	B	73	SER
2	B	113	ILE
2	B	131	LEU
2	B	133	LYS
2	B	134	MET
2	B	162	LYS
1	E	714	GLN
1	E	717	GLN
1	E	724	VAL
1	E	731	ARG
1	E	750	LEU
1	E	758	LEU
1	E	769	LEU
1	E	778	LEU
1	E	793	CYS
1	E	798	LYS
1	E	807	LYS
1	E	822	ARG
1	E	831	GLN
1	E	843	ILE
1	E	854	GLN
1	E	855	LEU
1	E	871	LEU
1	E	873	ASP
1	E	879	MET
1	E	884	LYS
1	E	887	LEU
1	E	888	LEU
1	E	940	LEU
1	E	945	LEU
1	E	957	LYS
1	E	964	ARG
1	E	965	LYS
1	E	967	ILE
1	E	973	THR
1	E	978	LYS

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Mol	Chain	Res	Type
1	E	981	THR
1	E	988	LEU
1	E	997	GLN
1	E	998	LYS
1	E	1004	LEU
1	E	1010	LYS
1	E	1036	VAL
1	E	1055	GLN
1	E	1056	ILE
1	E	1065	SER
1	E	1068	ASN
1	E	1074	LEU
2	F	4	ILE
2	F	8	LEU
2	F	11	VAL
2	F	21	LEU
2	F	28	ASP
2	F	32	GLU
2	F	35	VAL
2	F	55	LEU
2	F	113	ILE
2	F	131	LEU
2	F	134	MET
2	F	162	LYS
2	F	168	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	A	863	HIS
1	E	717	GLN
1	E	997	GLN
1	E	1008	HIS

### 5.3.3 RNA ⓘ

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, 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	355/418 (84%)	0.03	14 (3%) 43 32	38, 65, 108, 130	0
1	E	358/418 (85%)	0.04	16 (4%) 37 27	38, 66, 110, 133	0
2	B	178/178 (100%)	-0.02	6 (3%) 49 38	40, 58, 98, 114	0
2	F	178/178 (100%)	-0.01	6 (3%) 49 38	40, 61, 98, 112	0
All	All	1069/1192 (89%)	0.02	42 (3%) 43 32	38, 63, 106, 133	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1051	LEU	7.2
1	E	1053	PRO	6.5
1	E	1037	ALA	6.4
1	A	1054	PRO	4.6
2	F	32	GLU	4.3
1	A	1050	LYS	3.9
1	E	1052	GLY	3.8
2	B	135	LYS	3.6
1	A	720	VAL	3.6
1	A	1053	PRO	3.6
2	B	32	GLU	3.6
2	F	30	PHE	3.6
1	A	1048	THR	3.5
2	F	33	VAL	3.4
1	E	946	GLU	3.0
1	E	1038	THR	3.0
1	E	948	ALA	2.9
2	F	29	GLN	2.9
1	A	979	ASP	2.9
1	E	947	ARG	2.9
1	E	949	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	723	ASP	2.7
1	A	949	SER	2.7
1	A	721	GLY	2.7
1	E	720	VAL	2.6
1	A	948	ALA	2.6
1	E	979	ASP	2.6
2	F	31	PRO	2.5
1	E	721	GLY	2.4
1	E	723	ASP	2.3
1	E	958	SER	2.3
1	A	947	ARG	2.3
1	E	1047	CYS	2.2
2	B	126	HIS	2.2
1	A	1001	GLU	2.2
2	B	30	PHE	2.1
2	B	29	GLN	2.1
1	E	1080	ASN	2.1
1	A	1040	LYS	2.1
2	B	125	GLU	2.1
1	A	719	THR	2.1
2	F	28	ASP	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.