



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 5DFV / pdb\_00005dfv  
Title : CRYSTAL STRUCTURE OF HUMAN CD81 LARGE EXTRACELLULAR LOOP IN COMPLEX WITH MURINE FAB FRAGMENT K04  
Authors : Harris, S.F.; Wong, A.; Kuglstatter, A.  
Deposited on : 2015-08-27  
Resolution : 2.80 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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

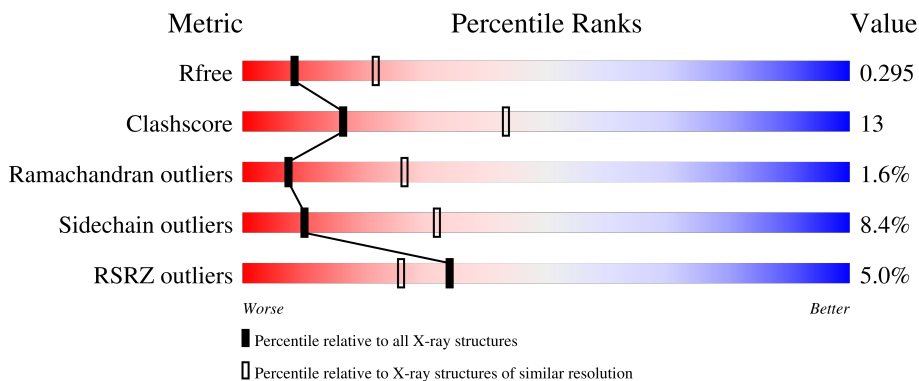
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



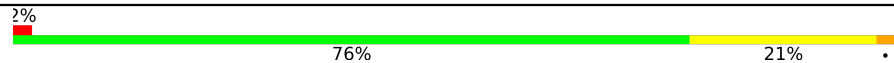
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	99	
1	B	99	
2	C	222	
2	E	222	
3	D	218	

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Mol	Chain	Length	Quality of chain
3	F	218	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '2%', a large green segment in the middle labeled '76%', and a yellow segment on the right labeled '21%'. A small black dot is visible at the far right end of the bar.</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7930 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 CD81 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	88	683	425	116	138	4	0	0	0
1	B	86	657	408	112	133	4	1	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	-	expression tag	UNP P60033
A	111	SER	-	expression tag	UNP P60033
A	202	HIS	LEU	conflict	UNP P60033
A	203	HIS	-	expression tag	UNP P60033
A	204	HIS	-	expression tag	UNP P60033
A	205	HIS	-	expression tag	UNP P60033
A	206	HIS	-	expression tag	UNP P60033
A	207	HIS	-	expression tag	UNP P60033
A	208	HIS	-	expression tag	UNP P60033
B	110	GLY	-	expression tag	UNP P60033
B	111	SER	-	expression tag	UNP P60033
B	202	HIS	LEU	conflict	UNP P60033
B	203	HIS	-	expression tag	UNP P60033
B	204	HIS	-	expression tag	UNP P60033
B	205	HIS	-	expression tag	UNP P60033
B	206	HIS	-	expression tag	UNP P60033
B	207	HIS	-	expression tag	UNP P60033
B	208	HIS	-	expression tag	UNP P60033

- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	214	1599	1011	268	314	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	214	Total	C	N	O	S	0	0	0
			1599	1011	268	314	6			

- Molecule 3 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1694	1061	284	343	6			
3	F	217	Total	C	N	O	S	0	0	0
			1694	1061	284	343	6			

- Molecule 4 is water.

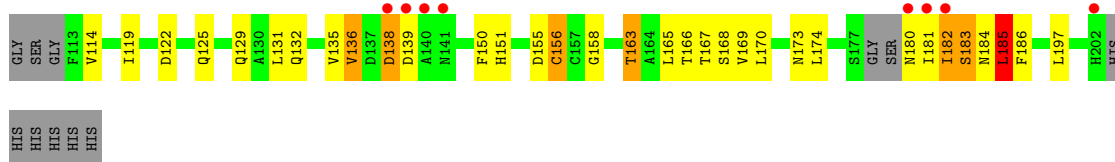
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		

### 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: CD81 antigen

Chain A: 



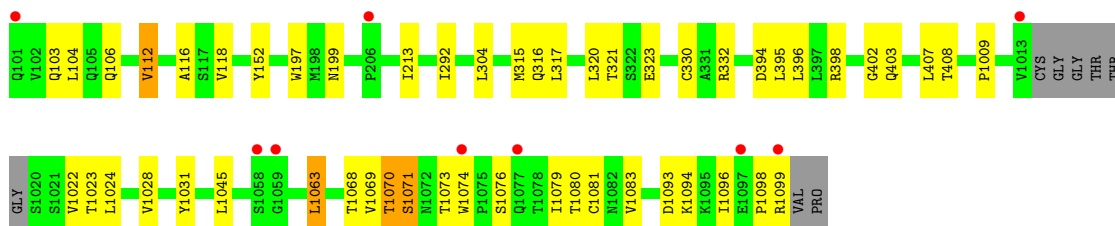
- Molecule 1: CD81 antigen

Chain B: 



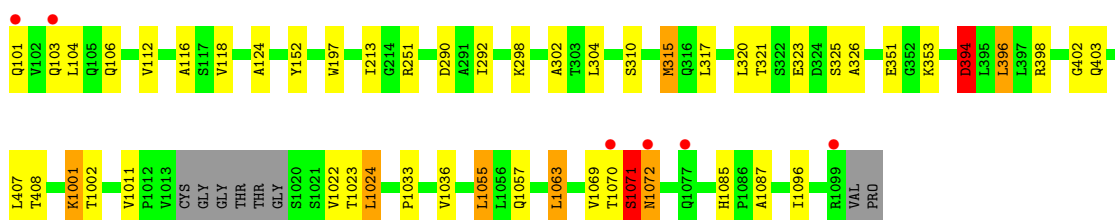
- Molecule 2: FAB HEAVY CHAIN

Chain C: 



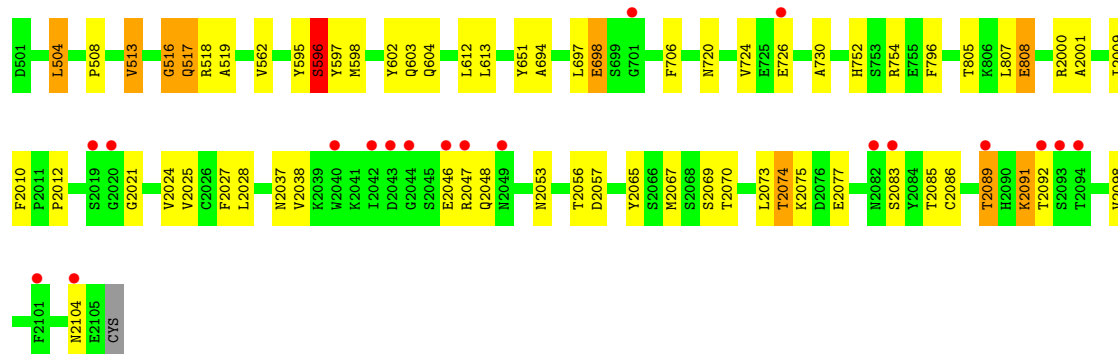
- Molecule 2: FAB HEAVY CHAIN

Chain E: 




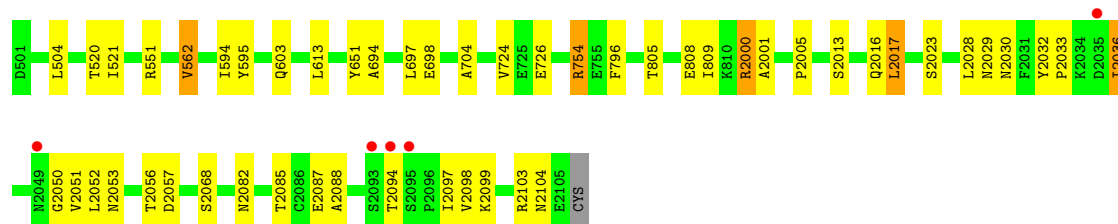
- Molecule 3: FAB LIGHT CHAIN

Chain D: 



- Molecule 3: FAB LIGHT CHAIN

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.63Å 94.48Å 94.11Å 90.00° 104.14° 90.00°	Depositor
Resolution (Å)	47.25 – 2.80 47.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (47.25-2.80) 93.9 (47.25-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.239 , 0.291 0.244 , 0.295	Depositor DCC
$R_{free}$ test set	1583 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 23.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	0.52	0/691	0.78	0/932
1	B	0.55	1/664 (0.2%)	0.80	1/895 (0.1%)
2	C	0.44	0/1636	0.72	0/2225
2	E	0.44	0/1636	0.71	2/2225 (0.1%)
3	D	0.42	0/1736	0.73	2/2358 (0.1%)
3	F	0.44	0/1736	0.66	0/2358
All	All	0.45	1/8099 (0.0%)	0.72	5/10993 (0.0%)

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
3	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	PHE	CA-CB	-7.44	1.38	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1071	SER	CA-C-N	6.15	132.76	121.70
2	E	1071	SER	C-N-CA	6.15	132.76	121.70
3	D	596	SER	CA-C-N	5.88	132.28	121.70
3	D	596	SER	C-N-CA	5.88	132.28	121.70
1	B	113	PHE	CB-CA-C	-5.12	100.37	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	596	SER	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	683	0	663	38	0
1	B	657	0	636	29	0
2	C	1599	0	1587	35	0
2	E	1599	0	1587	52	0
3	D	1694	0	1621	40	0
3	F	1694	0	1619	28	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
All	All	7930	0	7713	201	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 13.

All (201) 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)
2:E:118:VAL:HG23	2:E:320:LEU:HD11	1.28	1.15
1:B:167:THR:HG21	2:E:292:ILE:HD11	1.41	1.01
2:E:213:ILE:HD13	2:E:315:MET:CE	1.99	0.92
2:C:118:VAL:HG23	2:C:320:LEU:HD11	1.51	0.92
1:A:135:VAL:HG21	1:A:165:LEU:HD22	1.54	0.89
2:E:396:LEU:O	2:E:396:LEU:HD23	1.74	0.87
3:D:516:GLY:HA3	3:D:517:GLN:HB2	1.57	0.85
3:F:2028:LEU:HD23	3:F:2036:ILE:HD13	1.58	0.85
2:E:394:ASP:HB3	2:E:396:LEU:HD22	1.61	0.82
3:F:2056:THR:HG22	3:F:2057:ASP:O	1.80	0.81
2:E:213:ILE:HD13	2:E:315:MET:HE1	1.61	0.80
2:E:118:VAL:CG2	2:E:320:LEU:HD11	2.12	0.78
1:A:182:ILE:HG22	1:A:183:SER:N	2.00	0.76
2:E:396:LEU:HD21	2:E:398:ARG:HH21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:516:GLY:CA	3:D:517:GLN:HB2	2.16	0.75
2:C:1024:LEU:HD22	2:C:1096:ILE:HG21	1.68	0.75
2:E:213:ILE:HG21	2:E:315:MET:HE2	1.70	0.74
2:E:112:VAL:HG21	2:E:118:VAL:HG22	1.70	0.72
2:C:213:ILE:HD13	2:C:315:MET:HE1	1.72	0.71
2:E:1071:SER:H	2:E:1072:ASN:HB2	1.56	0.71
1:A:132:GLN:O	1:A:136:VAL:HG12	1.92	0.69
2:E:1071:SER:H	2:E:1072:ASN:CB	2.06	0.69
1:B:167:THR:HG21	2:E:292:ILE:CD1	2.22	0.69
3:D:504:LEU:HD11	3:D:598:MET:HE1	1.75	0.67
3:F:2088:ALA:HB3	3:F:2097:ILE:HG23	1.74	0.67
1:A:197:LEU:HD12	1:B:149:THR:HG22	1.76	0.67
2:E:394:ASP:CB	2:E:396:LEU:HD22	2.26	0.66
3:F:697:LEU:HD11	3:F:704:ALA:HA	1.78	0.66
2:E:1063:LEU:C	2:E:1063:LEU:HD12	2.22	0.65
1:A:163:THR:O	1:A:166:THR:HG22	1.97	0.65
3:D:604:GLN:O	3:D:730:ALA:HB1	1.95	0.65
2:E:1055:LEU:HD23	3:F:2052:LEU:HB3	1.77	0.65
2:E:213:ILE:HD13	2:E:315:MET:HE3	1.79	0.64
1:A:114:VAL:HG11	1:A:119:ILE:CD1	2.28	0.64
3:D:596:SER:HA	3:D:597:TYR:HB2	1.79	0.64
3:D:2091:LYS:HD2	3:D:2092:THR:HG23	1.80	0.62
1:B:167:THR:CG2	2:E:292:ILE:HD11	2.25	0.62
2:C:395:LEU:C	2:C:396:LEU:HD12	2.25	0.62
2:C:1009:PRO:HB3	2:C:1096:ILE:HD13	1.81	0.61
1:A:167:THR:HG21	2:C:292:ILE:HD11	1.83	0.61
2:C:112:VAL:HG11	2:C:118:VAL:CG2	2.31	0.61
3:D:513:VAL:HG21	3:D:519:ALA:HB2	1.85	0.59
2:E:396:LEU:HD23	2:E:396:LEU:C	2.28	0.59
2:C:1023:THR:HB	2:C:1068:THR:HG22	1.84	0.58
2:E:1011:VAL:HA	2:E:1096:ILE:HD11	1.83	0.58
3:D:603:GLN:HB2	3:D:613:LEU:HD11	1.85	0.58
3:F:2013:SER:O	3:F:2017:LEU:HD22	2.04	0.58
1:A:131:LEU:CD1	1:A:169:VAL:HG21	2.34	0.58
1:A:114:VAL:CG1	1:A:119:ILE:CD1	2.82	0.58
1:A:114:VAL:CG1	1:A:119:ILE:HD11	2.33	0.58
3:F:724:VAL:CG1	3:F:809:ILE:HD12	2.34	0.58
2:C:1070:THR:HG21	2:C:1073:THR:HG23	1.85	0.57
2:C:1028:VAL:HG22	2:C:1083:VAL:HG21	1.85	0.57
2:E:292:ILE:HD13	3:F:796:PHE:CZ	2.41	0.56
1:A:114:VAL:HG11	1:A:119:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLN:HE21	2:C:402:GLY:HA3	1.71	0.56
2:C:1069:VAL:HG12	2:C:1070:THR:HG22	1.88	0.55
1:B:131:LEU:HD12	1:B:169:VAL:HG11	1.87	0.55
1:A:122:ASP:HB3	1:B:119:ILE:HD13	1.88	0.55
3:F:2087:GLU:HG2	3:F:2098:VAL:HG22	1.88	0.55
2:C:1080:THR:HG23	2:C:1094:LYS:C	2.32	0.55
1:B:182:ILE:HG21	2:E:290:ASP:OD2	2.06	0.55
1:A:183:SER:HA	1:A:185:LEU:N	2.23	0.54
2:E:1069:VAL:HG22	2:E:1070:THR:H	1.72	0.54
1:A:183:SER:HA	1:A:184:ASN:C	2.32	0.53
3:F:2000:ARG:HD3	3:F:2001:ALA:O	2.09	0.53
2:C:1023:THR:HG22	2:C:1068:THR:HB	1.90	0.53
2:E:1024:LEU:HB2	2:E:1096:ILE:HD13	1.89	0.53
1:B:131:LEU:CD1	1:B:169:VAL:HG11	2.38	0.53
1:B:132:GLN:O	1:B:136:VAL:HG13	2.08	0.53
2:C:112:VAL:HG11	2:C:118:VAL:HG22	1.90	0.53
3:F:594:ILE:HD12	3:F:595:TYR:CE1	2.43	0.53
3:F:2005:PRO:HG3	3:F:2036:ILE:HD11	1.91	0.53
1:B:166:THR:HA	1:B:169:VAL:HG22	1.90	0.53
2:E:321:THR:HG22	2:E:323:GLU:H	1.75	0.52
3:D:562:VAL:HG23	3:D:754:ARG:HB2	1.90	0.52
3:D:517:GLN:O	3:D:724:VAL:HG23	2.09	0.52
1:B:158:GLY:HA3	1:B:166:THR:HG23	1.91	0.52
1:B:170:LEU:C	1:B:170:LEU:HD23	2.35	0.52
1:A:182:ILE:CG2	1:A:183:SER:N	2.73	0.51
1:A:136:VAL:HG11	3:D:595:TYR:CE1	2.46	0.51
1:B:160:SER:O	1:B:163:THR:HG22	2.10	0.51
1:A:163:THR:HA	1:A:166:THR:HG22	1.93	0.51
3:D:2074:THR:HG23	3:D:2077:GLU:CB	2.41	0.51
1:A:158:GLY:HA3	1:A:166:THR:OG1	2.09	0.51
1:B:197:LEU:C	1:B:197:LEU:HD23	2.36	0.51
3:D:808:GLU:HG2	3:D:2065:TYR:OH	2.11	0.51
3:D:651:TYR:O	3:D:694:ALA:HB3	2.11	0.51
3:D:2037:ASN:HB3	3:D:2089:THR:HG22	1.93	0.51
3:F:2082:ASN:ND2	3:F:2103:ARG:O	2.44	0.51
1:A:135:VAL:CG2	1:A:165:LEU:HD22	2.33	0.50
1:B:158:GLY:O	1:B:190:CYS:HB3	2.11	0.50
1:A:150:PHE:CZ	1:B:197:LEU:HD21	2.46	0.50
3:D:2012:PRO:HD3	3:D:2024:VAL:HG22	1.93	0.50
1:A:163:THR:C	1:A:166:THR:HG22	2.36	0.50
3:D:562:VAL:HG21	3:D:752:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:HA3	1:B:166:THR:CG2	2.42	0.50
2:C:1031:TYR:OH	2:C:1063:LEU:HD23	2.12	0.50
3:D:697:LEU:HD21	3:D:706:PHE:O	2.12	0.50
1:A:114:VAL:H	1:B:129:GLN:HE22	1.59	0.49
1:A:173:ASN:O	1:A:174:LEU:HD23	2.12	0.49
2:E:1022:VAL:HG23	2:E:1071:SER:HB2	1.94	0.49
1:A:114:VAL:HG11	1:A:119:ILE:HD12	1.93	0.49
2:C:1098:PRO:O	2:C:1099:ARG:C	2.56	0.49
1:B:201:LYS:O	1:B:202:HIS:C	2.55	0.49
3:D:2025:VAL:HG22	3:D:2070:THR:HG23	1.93	0.49
1:B:182:ILE:HG21	2:E:290:ASP:CG	2.37	0.49
3:D:513:VAL:HG11	3:D:518:ARG:O	2.12	0.49
2:C:394:ASP:O	2:C:396:LEU:N	2.42	0.49
2:C:321:THR:HG22	2:C:323:GLU:H	1.78	0.49
2:E:103:GLN:C	2:E:104:LEU:HD12	2.38	0.49
3:F:2052:LEU:C	3:F:2053:ASN:HD22	2.19	0.49
1:B:139:ASP:O	1:B:141:ASN:N	2.46	0.48
2:C:104:LEU:HD23	2:C:330:CYS:SG	2.54	0.48
3:D:2009:ILE:HD11	3:D:2086:CYS:CB	2.43	0.48
1:A:182:ILE:HG22	1:A:183:SER:H	1.73	0.48
1:B:167:THR:HG22	2:E:197:TRP:CH2	2.49	0.48
2:E:124:ALA:HB1	2:E:152:TYR:CE1	2.48	0.48
2:E:325:SER:O	2:E:326:ALA:HB2	2.14	0.48
1:B:170:LEU:HD12	1:B:185:LEU:HD21	1.95	0.48
3:D:2038:VAL:CG2	3:D:2067:MET:HE1	2.44	0.47
3:D:2073:LEU:HD12	3:D:2074:THR:O	2.14	0.47
2:E:1070:THR:O	2:E:1070:THR:HG23	2.15	0.47
3:F:562:VAL:O	3:F:562:VAL:CG1	2.61	0.47
3:F:2028:LEU:HD12	3:F:2028:LEU:N	2.30	0.47
3:D:612:LEU:HD23	3:D:698:GLU:HG3	1.96	0.47
1:B:167:THR:HG22	2:E:197:TRP:CZ2	2.50	0.46
3:D:2085:THR:HG23	3:D:2098:VAL:HG12	1.97	0.46
2:E:353:LYS:H	2:E:353:LYS:HD2	1.80	0.46
3:D:562:VAL:O	3:D:562:VAL:HG22	2.14	0.46
3:D:2085:THR:CG2	3:D:2098:VAL:HG12	2.46	0.46
1:A:131:LEU:HD12	1:A:169:VAL:HG21	1.96	0.46
3:F:651:TYR:O	3:F:694:ALA:HB3	2.16	0.46
2:C:1070:THR:HG22	2:C:1073:THR:OG1	2.16	0.46
3:D:562:VAL:O	3:D:597:TYR:HB2	2.16	0.46
3:D:2038:VAL:HG23	3:D:2067:MET:HE1	1.98	0.46
2:E:1085:HIS:CE1	2:E:1087:ALA:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:MET:HE2	2:C:317:LEU:HD11	1.97	0.46
1:A:167:THR:HG22	2:C:197:TRP:CZ2	2.50	0.46
2:C:118:VAL:HG21	2:C:407:LEU:HD21	1.97	0.45
1:B:182:ILE:HG21	2:E:290:ASP:OD1	2.16	0.45
3:F:2088:ALA:HB3	3:F:2097:ILE:CG2	2.44	0.45
1:A:184:ASN:O	1:A:186:PHE:N	2.50	0.45
2:C:292:ILE:HD13	3:D:796:PHE:CE1	2.51	0.45
2:E:1070:THR:HA	2:E:1071:SER:CB	2.47	0.45
1:A:151:HIS:HA	1:A:156:CYS:HB3	1.99	0.44
1:A:136:VAL:HG23	3:D:651:TYR:CE2	2.52	0.44
1:B:182:ILE:CG2	2:E:290:ASP:OD2	2.65	0.44
2:C:1009:PRO:CB	2:C:1096:ILE:HD13	2.47	0.44
3:F:2028:LEU:HD23	3:F:2036:ILE:CD1	2.40	0.44
1:A:125:GLN:O	1:A:129:GLN:HG3	2.17	0.44
1:A:151:HIS:ND1	1:A:174:LEU:O	2.50	0.44
2:E:1071:SER:H	2:E:1072:ASN:CA	2.31	0.44
1:A:131:LEU:HD11	1:A:169:VAL:HG21	2.00	0.44
3:D:2027:PHE:C	3:D:2028:LEU:HD12	2.42	0.44
1:B:140:ALA:HB1	1:B:143:ALA:HB3	2.00	0.44
2:C:152:TYR:CZ	2:C:332:ARG:HD2	2.52	0.44
3:F:521:ILE:HG12	3:F:805:THR:HG21	1.98	0.44
2:C:1080:THR:HG21	2:C:1093:ASP:HB3	1.99	0.44
3:D:2074:THR:HG23	3:D:2077:GLU:HB3	1.98	0.44
3:F:2056:THR:CG2	3:F:2057:ASP:N	2.80	0.44
3:D:516:GLY:HA3	3:D:517:GLN:HE21	1.83	0.44
3:D:2009:ILE:HG22	3:D:2010:PHE:N	2.33	0.44
3:F:2016:GLN:HE22	3:F:2023:SER:CB	2.31	0.44
3:D:508:PRO:O	3:D:805:THR:HG23	2.18	0.43
3:D:596:SER:HA	3:D:597:TYR:CB	2.47	0.43
2:E:251:ARG:HD2	2:E:351:GLU:OE2	2.18	0.43
1:A:114:VAL:CG1	1:A:119:ILE:HD12	2.48	0.43
2:C:1070:THR:O	2:C:1071:SER:CB	2.66	0.43
1:A:138:ASP:CG	1:A:138:ASP:O	2.62	0.43
2:E:302:ALA:HA	2:E:317:LEU:HD23	1.99	0.43
1:A:180:ASN:O	1:A:181:ILE:HG23	2.19	0.43
2:E:1070:THR:OG1	2:E:1071:SER:HB3	2.18	0.43
2:E:112:VAL:HG11	2:E:320:LEU:HD12	2.00	0.43
2:E:1072:ASN:N	2:E:1072:ASN:OD1	2.52	0.43
1:A:163:THR:HA	1:A:166:THR:CG2	2.48	0.42
2:E:1033:PRO:HD2	2:E:1087:ALA:CB	2.49	0.42
2:E:106:GLN:HE21	2:E:402:GLY:HA3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:VAL:HG23	2:C:116:ALA:HB3	2.00	0.42
2:C:1022:VAL:HG11	2:C:1074:TRP:HB3	2.01	0.42
2:E:112:VAL:CG1	2:E:116:ALA:HB3	2.50	0.42
3:F:754:ARG:HD2	3:F:754:ARG:O	2.20	0.42
3:D:2056:THR:HG22	3:D:2057:ASP:N	2.34	0.42
3:F:2000:ARG:CD	3:F:2001:ALA:O	2.67	0.42
2:E:1002:THR:HG21	2:E:1087:ALA:O	2.20	0.41
3:F:603:GLN:HB2	3:F:613:LEU:HD11	2.02	0.41
3:F:2028:LEU:HD22	3:F:2036:ILE:HG21	2.02	0.41
2:C:103:GLN:C	2:C:104:LEU:HD12	2.45	0.41
2:C:1069:VAL:HG21	2:C:1079:ILE:CD1	2.49	0.41
2:E:1001:LYS:CD	2:E:1001:LYS:N	2.83	0.41
2:E:1024:LEU:CB	2:E:1096:ILE:HD13	2.50	0.41
2:E:1024:LEU:CD1	2:E:1096:ILE:HG21	2.50	0.41
1:A:125:GLN:HG2	1:B:114:VAL:HG21	2.02	0.41
1:B:160:SER:O	1:B:163:THR:CG2	2.69	0.41
2:C:118:VAL:HG23	2:C:320:LEU:CD1	2.37	0.41
2:C:112:VAL:HG11	2:C:118:VAL:HG21	2.01	0.40
3:D:602:TYR:CZ	3:D:612:LEU:HD13	2.56	0.40
3:D:2009:ILE:CG2	3:D:2010:PHE:N	2.84	0.40
3:F:2029:ASN:HB3	3:F:2030:ASN:HD22	1.86	0.40
3:F:2032:TYR:CG	3:F:2033:PRO:HA	2.56	0.40
2:E:213:ILE:HG21	2:E:315:MET:CE	2.47	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	84/99 (85%)	73 (87%)	6 (7%)	5 (6%)	<b>1</b> <b>3</b>
1	B	82/99 (83%)	76 (93%)	5 (6%)	1 (1%)	<b>10</b> <b>34</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	210/222 (95%)	195 (93%)	13 (6%)	2 (1%)	12	38
2	E	210/222 (95%)	192 (91%)	16 (8%)	2 (1%)	12	38
3	D	215/218 (99%)	185 (86%)	26 (12%)	4 (2%)	6	22
3	F	215/218 (99%)	203 (94%)	10 (5%)	2 (1%)	14	41
All	All	1016/1078 (94%)	924 (91%)	76 (8%)	16 (2%)	7	27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	185	LEU
1	B	140	ALA
3	D	517	GLN
3	D	2001	ALA
2	C	1071	SER
3	D	2021	GLY
2	E	1071	SER
1	A	139	ASP
2	C	1070	THR
1	A	138	ASP
1	A	155	ASP
3	D	516	GLY
3	F	2104	ASN
2	E	394	ASP
3	F	2050	GLY

### 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	79/87 (91%)	72 (91%)	7 (9%)	9	29
1	B	75/87 (86%)	71 (95%)	4 (5%)	20	52
2	C	180/186 (97%)	169 (94%)	11 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	180/186 (97%)	161 (89%)	19 (11%)	6	22
3	D	193/194 (100%)	174 (90%)	19 (10%)	7	25
3	F	193/194 (100%)	177 (92%)	16 (8%)	10	32
All	All	900/934 (96%)	824 (92%)	76 (8%)	10	32

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	156	CYS
1	A	163	THR
1	A	168	SER
1	A	170	LEU
1	A	183	SER
1	A	185	LEU
1	B	136	VAL
1	B	160	SER
1	B	163	THR
1	B	202	HIS
2	C	112	VAL
2	C	199	ASN
2	C	304	LEU
2	C	316	GLN
2	C	398	ARG
2	C	403	GLN
2	C	408	THR
2	C	1045	LEU
2	C	1063	LEU
2	C	1076	SER
2	C	1081	CYS
3	D	504	LEU
3	D	513	VAL
3	D	698	GLU
3	D	720	ASN
3	D	726	GLU
3	D	807	LEU
3	D	808	GLU
3	D	2000	ARG
3	D	2046	GLU
3	D	2047	ARG
3	D	2048	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	2053	ASN
3	D	2069	SER
3	D	2074	THR
3	D	2075	LYS
3	D	2083	SER
3	D	2089	THR
3	D	2091	LYS
3	D	2104	ASN
2	E	101	GLN
2	E	298	LYS
2	E	304	LEU
2	E	310	SER
2	E	315	MET
2	E	394	ASP
2	E	396	LEU
2	E	403	GLN
2	E	407	LEU
2	E	408	THR
2	E	1001	LYS
2	E	1023	THR
2	E	1024	LEU
2	E	1036	VAL
2	E	1055	LEU
2	E	1057	GLN
2	E	1063	LEU
2	E	1071	SER
2	E	1072	ASN
3	F	504	LEU
3	F	520	THR
3	F	551	ARG
3	F	562	VAL
3	F	698	GLU
3	F	726	GLU
3	F	754	ARG
3	F	808	GLU
3	F	2000	ARG
3	F	2017	LEU
3	F	2036	ILE
3	F	2051	VAL
3	F	2068	SER
3	F	2085	THR
3	F	2094	THR

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Mol	Chain	Res	Type
3	F	2099	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	184	ASN
1	B	172	ASN
2	C	105	GLN
2	C	106	GLN
2	C	204	GLN
2	C	1077	GLN
3	D	517	GLN
3	D	603	GLN
3	D	604	GLN
3	D	608	GLN
3	D	722	HIS
3	D	2037	ASN
3	D	2048	GLN
3	D	2053	ASN
3	D	2058	GLN
3	D	2082	ASN
3	D	2104	ASN
2	E	103	GLN
2	E	106	GLN
2	E	1085	HIS
3	F	2030	ASN
3	F	2053	ASN

### 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 oligosaccharides 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	88/99 (88%)	0.64	8 (9%) 15 11	27, 35, 44, 50	0
1	B	86/99 (86%)	0.37	5 (5%) 29 22	22, 32, 41, 42	1 (1%)
2	C	214/222 (96%)	0.44	9 (4%) 40 32	23, 30, 49, 56	0
2	E	214/222 (96%)	0.29	6 (2%) 55 45	18, 25, 46, 51	0
3	D	217/218 (99%)	0.77	19 (8%) 15 11	24, 42, 68, 70	0
3	F	217/218 (99%)	0.13	5 (2%) 61 51	17, 25, 47, 53	0
All	All	1036/1078 (96%)	0.42	52 (5%) 34 26	17, 32, 58, 70	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	101	GLN	4.0
1	B	113	PHE	3.8
1	A	140	ALA	3.7
2	C	101	GLN	3.6
3	F	2094	THR	3.4
3	D	2049	ASN	3.4
1	A	180	ASN	3.3
1	A	139	ASP	3.3
2	E	1099	ARG	3.2
3	D	2094	THR	3.1
2	C	1013	VAL	3.1
3	D	2104	ASN	3.0
3	D	726	GLU	3.0
3	F	2093	SER	3.0
2	C	206	PRO	3.0
3	D	2047	ARG	2.9
2	E	1077	GLN	2.8
2	C	1059	GLY	2.8
3	D	2042	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	138	ASP	2.7
3	D	701	GLY	2.6
1	A	202	HIS	2.6
1	A	141	ASN	2.6
2	E	1072	ASN	2.5
1	A	138	ASP	2.5
3	F	2095	SER	2.5
3	D	2092	THR	2.5
3	D	2019	SER	2.5
3	D	2044	GLY	2.5
1	A	182	ILE	2.4
1	B	139	ASP	2.4
1	B	182	ILE	2.4
2	C	1097	GLU	2.4
3	D	2043	ASP	2.3
3	D	2083	SER	2.3
2	E	1070	THR	2.2
3	D	2046	GLU	2.2
2	C	1099	ARG	2.2
3	D	2082	ASN	2.2
3	D	2101	PHE	2.2
3	D	2020	GLY	2.1
3	D	2040	TRP	2.1
3	D	2093	SER	2.1
2	C	1077	GLN	2.1
3	F	2049	ASN	2.1
1	A	181	ILE	2.1
1	B	141	ASN	2.0
3	D	2089	THR	2.0
3	F	2035	ASP	2.0
2	C	1058	SER	2.0
2	E	103	GLN	2.0
2	C	1074	TRP	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 oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.