



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3R08
Title : Crystal structure of mouse cd3epsilon in complex with antibody 2C11 Fab
Authors : Shore, D.A.; Zhu, X.; Wilson, I.A.
Deposited on : 2011-03-07
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

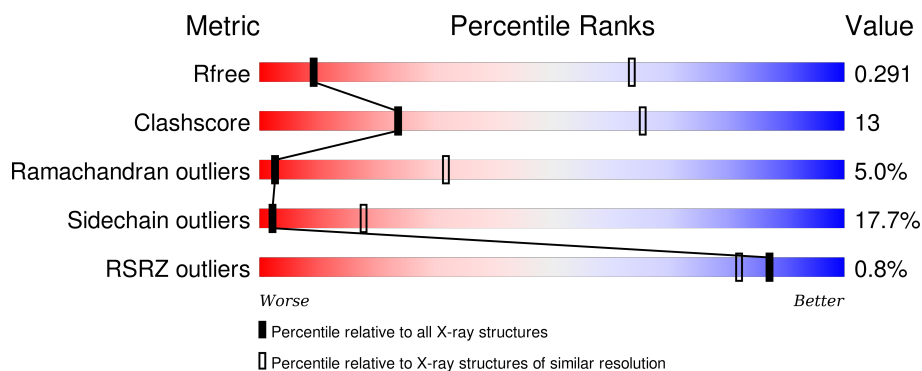
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	L	213	<div> <div></div> <div>54%37%9%</div> </div>
2	H	216	<div> <div>%</div> <div>61%34%5%</div> </div>
3	E	82	<div> <div>%</div> <div>57%34%9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3944 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 Mouse anti-mouse CD3epsilon antibody 2C11 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1664	1041	278	340	5			

- Molecule 2 is a protein called Mouse anti-mouse CD3epsilon antibody 2C11 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1626	1029	268	320	9			

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	82	Total	C	N	O	S	0	0	0
			654	410	105	137	2			

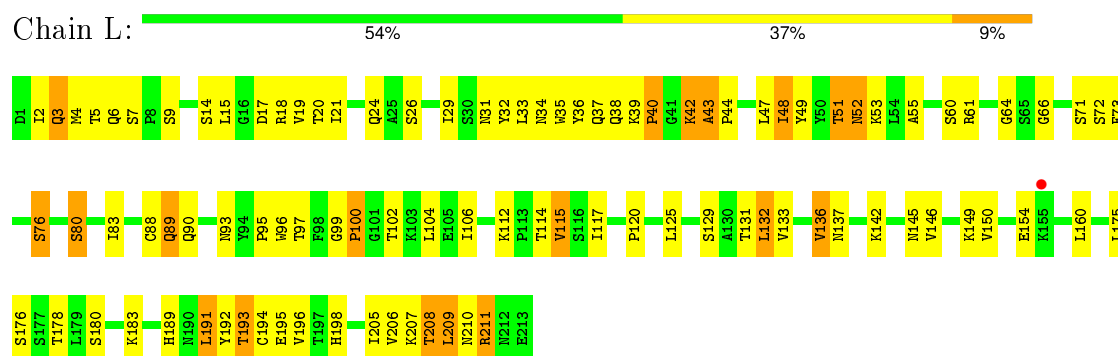
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	80	SER	-	EXPRESSION TAG	UNP P22646
E	81	GLU	-	EXPRESSION TAG	UNP P22646
E	82	TYR	-	EXPRESSION TAG	UNP P22646

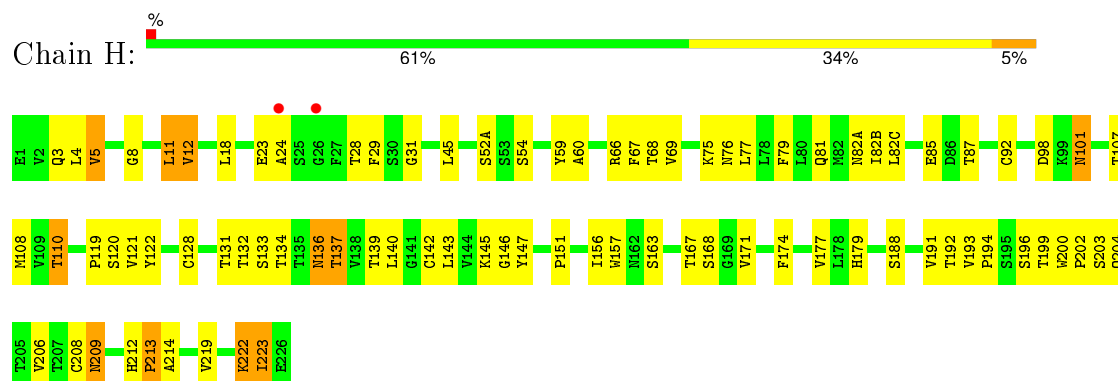
3 Residue-property plots

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.

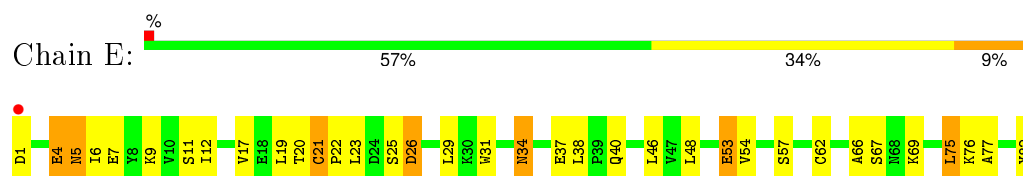
- Molecule 1: Mouse anti-mouse CD3epsilon antibody 2C11 light chain



- Molecule 2: Mouse anti-mouse CD3epsilon antibody 2C11 heavy chain



- Molecule 3: T-cell surface glycoprotein CD3 epsilon chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	263.18 Å 263.18 Å 263.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.15 – 4.10 43.86 – 4.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.15-4.10) 96.9 (43.86-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 4.13 Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.222 , 0.277 0.239 , 0.291	Depositor DCC
R_{free} test set	584 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	158.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 184.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 12126 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3944	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	L	0.54	0/1701	0.85	1/2309 (0.0%)
2	H	0.51	0/1666	0.83	0/2274
3	E	0.64	1/667 (0.1%)	0.98	0/904
All	All	0.54	1/4034 (0.0%)	0.87	1/5487 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	82	TYR	CB-CG	-6.09	1.42	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	40	PRO	N-CA-C	5.51	126.43	112.10

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	L	1664	0	1608	52	0
2	H	1626	0	1593	41	0
3	E	654	0	612	13	0
All	All	3944	0	3813	102	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 (102) 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:H:156:ILE:HG13	2:H:209:ASN:HB2	1.62	0.82
2:H:151:PRO:HD2	2:H:213:PRO:HG3	1.66	0.77
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.67	0.75
2:H:133:SER:HB2	2:H:136:ASN:HA	1.70	0.74
3:E:9:LYS:HB3	3:E:20:THR:HB	1.72	0.72
1:L:34:ASN:HD22	1:L:49:TYR:HA	1.56	0.71
2:H:171:VAL:HG22	2:H:191:VAL:HG23	1.71	0.71
1:L:115:VAL:HG21	1:L:196:VAL:HG21	1.74	0.68
2:H:206:VAL:H	2:H:222:LYS:HE3	1.59	0.68
1:L:90:GLN:HE21	1:L:97:THR:H	1.47	0.62
1:L:189:HIS:O	1:L:211:ARG:NH1	2.32	0.62
1:L:4:MET:HB2	1:L:99:GLY:HA2	1.82	0.62
1:L:120:PRO:HD3	1:L:132:LEU:HG	1.80	0.61
1:L:193:THR:HG23	1:L:208:THR:HG23	1.81	0.61
1:L:52:ASN:H	1:L:52:ASN:HD22	1.48	0.60
2:H:68:THR:HG23	2:H:81:GLN:HB3	1.84	0.60
2:H:5:VAL:HG23	2:H:23:GLU:HB2	1.84	0.60
2:H:87:THR:HG23	2:H:110:THR:HA	1.84	0.59
1:L:83:ILE:HG12	1:L:106:ILE:HB	1.86	0.58
1:L:66:GLY:HA3	1:L:71:SER:HA	1.85	0.58
1:L:15:LEU:HD11	1:L:106:ILE:HD11	1.86	0.57
1:L:36:TYR:OH	1:L:89:GLN:NE2	2.38	0.57
1:L:195:GLU:HA	1:L:206:VAL:HG12	1.86	0.56
1:L:115:VAL:CG2	1:L:196:VAL:HG21	2.34	0.56
3:E:7:GLU:HA	3:E:22:PRO:HB3	1.86	0.56
2:H:66:ARG:HD3	2:H:82(B):ILE:O	2.04	0.56
1:L:2:ILE:HG22	1:L:3:GLN:N	2.20	0.56
1:L:21:ILE:HG12	1:L:102:THR:HG21	1.89	0.55
1:L:95:PRO:HG3	2:H:60:ALA:HA	1.89	0.55
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.89	0.54
2:H:212:HIS:HE1	2:H:214:ALA:HB3	1.71	0.54
2:H:29:PHE:HB3	2:H:76:ASN:HD22	1.72	0.54
3:E:29:LEU:HD11	3:E:62:CYS:SG	2.47	0.53
1:L:37:GLN:HB2	1:L:47:LEU:HD21	1.89	0.53
1:L:6:GLN:HB2	1:L:100:PRO:HD2	1.88	0.53
1:L:34:ASN:ND2	1:L:49:TYR:HA	2.23	0.53
3:E:75:LEU:O	3:E:76:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:ASN:HD21	2:H:174:PHE:HZ	1.57	0.53
1:L:136:VAL:HG23	1:L:175:LEU:HB3	1.90	0.52
1:L:42:LYS:HE3	1:L:42:LYS:H	1.74	0.52
1:L:146:VAL:HG12	1:L:196:VAL:HA	1.91	0.52
2:H:133:SER:CB	2:H:136:ASN:HA	2.40	0.52
2:H:66:ARG:HG3	2:H:67:PHE:CD1	2.46	0.52
2:H:66:ARG:HG3	2:H:67:PHE:HD1	1.74	0.51
2:H:31:GLY:HA2	2:H:52(A):SER:HB2	1.92	0.51
2:H:212:HIS:CE1	2:H:214:ALA:HB3	2.46	0.51
1:L:6:GLN:NE2	1:L:102:THR:H	2.09	0.50
2:H:11:LEU:HG	2:H:12:VAL:H	1.77	0.50
1:L:19:VAL:HG11	1:L:104:LEU:HD11	1.93	0.50
1:L:2:ILE:HG22	1:L:3:GLN:H	1.75	0.50
2:H:75:LYS:HB2	2:H:77:LEU:HD12	1.94	0.48
3:E:53:GLU:HG2	3:E:76:LYS:HB2	1.95	0.48
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.49	0.48
1:L:5:THR:HB	1:L:24:GLN:HB3	1.95	0.47
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.97	0.47
1:L:150:VAL:HG22	1:L:192:TYR:HD1	1.80	0.46
2:H:157:TRP:CH2	2:H:208:CYS:HB2	2.51	0.46
3:E:67:SER:C	3:E:69:LYS:H	2.19	0.46
2:H:120:SER:HB3	2:H:122:TYR:CZ	2.51	0.45
2:H:82(A):ASN:HB2	2:H:82(B):ILE:HD12	1.98	0.45
2:H:142:CYS:HB2	2:H:157:TRP:CZ2	2.52	0.45
1:L:43:ALA:HA	1:L:44:PRO:HD3	1.88	0.45
1:L:48:ILE:HG22	1:L:53:LYS:O	2.16	0.45
3:E:21:CYS:HB2	3:E:31:TRP:CZ2	2.52	0.45
1:L:48:ILE:HD12	1:L:64:GLY:N	2.32	0.45
1:L:131:THR:HG23	1:L:180:SER:HA	1.99	0.44
1:L:150:VAL:HG22	1:L:192:TYR:CD1	2.52	0.44
3:E:21:CYS:SG	3:E:22:PRO:HD2	2.58	0.44
1:L:49:TYR:HE1	1:L:55:ALA:HA	1.82	0.44
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.99	0.44
2:H:59:TYR:HE1	2:H:69:VAL:HG12	1.81	0.44
3:E:12:ILE:HG13	3:E:17:VAL:HG13	2.00	0.44
2:H:120:SER:HB2	2:H:145:LYS:HB3	1.99	0.44
1:L:209:LEU:HG	2:H:128:CYS:HB2	2.00	0.44
2:H:121:VAL:HB	2:H:219:VAL:HG11	1.99	0.43
1:L:196:VAL:HB	1:L:205:ILE:O	2.19	0.43
1:L:150:VAL:HG13	1:L:192:TYR:CE1	2.53	0.43
2:H:200:TRP:CD1	2:H:202:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:LEU:HD22	2:H:223:ILE:HD13	2.01	0.43
3:E:46:LEU:HD23	3:E:48:LEU:HD11	1.99	0.43
2:H:156:ILE:HD12	2:H:163:SER:HA	2.01	0.42
1:L:117:ILE:HD13	1:L:194:CYS:HB2	2.02	0.42
1:L:29:ILE:HD12	1:L:31:ASN:H	1.84	0.42
3:E:57:SER:OG	3:E:76:LYS:HB3	2.20	0.42
2:H:133:SER:HB2	2:H:136:ASN:CA	2.44	0.41
2:H:200:TRP:CG	2:H:202:PRO:HA	2.55	0.41
1:L:61:ARG:HB2	1:L:76:SER:HB3	2.02	0.41
3:E:4:GLU:HB3	3:E:5:ASN:H	1.69	0.41
1:L:2:ILE:CG2	1:L:3:GLN:N	2.84	0.41
1:L:52:ASN:H	1:L:52:ASN:ND2	2.15	0.41
1:L:125:LEU:O	1:L:183:LYS:HD2	2.21	0.41
2:H:157:TRP:CZ3	2:H:208:CYS:HB2	2.55	0.41
1:L:160:LEU:HD21	2:H:179:HIS:HB2	2.01	0.41
2:H:137:THR:HA	2:H:194:PRO:HA	2.03	0.41
1:L:191:LEU:HD12	1:L:210:ASN:HB2	2.02	0.41
3:E:31:TRP:HB3	3:E:38:LEU:HD12	2.03	0.40
1:L:193:THR:HG22	1:L:206:VAL:HB	2.04	0.40
1:L:48:ILE:HD11	1:L:73:PHE:HE1	1.87	0.40
2:H:199:THR:HA	2:H:204:GLN:NE2	2.37	0.40
1:L:2:ILE:CG2	1:L:3:GLN:H	2.34	0.40
2:H:101:ASN:HD22	2:H:101:ASN:HA	1.52	0.40
1:L:207:LYS:HA	1:L:207:LYS:HD2	2.01	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	L	211/213 (99%)	179 (85%)	22 (10%)	10 (5%)	3 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	214/216 (99%)	180 (84%)	27 (13%)	7 (3%)	5	43
3	E	80/82 (98%)	61 (76%)	11 (14%)	8 (10%)	1	13
All	All	505/511 (99%)	420 (83%)	60 (12%)	25 (5%)	3	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	18	ARG
1	L	40	PRO
1	L	43	ALA
1	L	51	THR
2	H	132	THR
2	H	136	ASN
3	E	26	ASP
1	L	60	SER
1	L	80	SER
1	L	211	ARG
2	H	146	GLY
1	L	26	SER
1	L	32	TYR
1	L	100	PRO
2	H	28	THR
3	E	6	ILE
3	E	77	ALA
2	H	131	THR
3	E	34	ASN
3	E	66	ALA
2	H	213	PRO
3	E	4	GLU
3	E	23	LEU
3	E	40	GLN
2	H	8	GLY

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	L	190/190 (100%)	153 (80%)	37 (20%)	2	14
2	H	184/184 (100%)	154 (84%)	30 (16%)	3	22
3	E	73/76 (96%)	61 (84%)	12 (16%)	3	21
All	All	447/450 (99%)	368 (82%)	79 (18%)	2	18

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	7	SER
1	L	9	SER
1	L	14	SER
1	L	17	ASP
1	L	20	THR
1	L	33	LEU
1	L	38	GLN
1	L	39	LYS
1	L	42	LYS
1	L	48	ILE
1	L	51	THR
1	L	52	ASN
1	L	72	SER
1	L	76	SER
1	L	80	SER
1	L	89	GLN
1	L	93	ASN
1	L	96	TRP
1	L	112	LYS
1	L	114	THR
1	L	115	VAL
1	L	129	SER
1	L	132	LEU
1	L	133	VAL
1	L	136	VAL
1	L	142	LYS
1	L	145	ASN
1	L	149	LYS
1	L	154	GLU
1	L	176	SER
1	L	178	THR
1	L	191	LEU
1	L	193	THR

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Mol	Chain	Res	Type
1	L	198	HIS
1	L	208	THR
1	L	209	LEU
2	H	3	GLN
2	H	5	VAL
2	H	11	LEU
2	H	12	VAL
2	H	18	LEU
2	H	45	LEU
2	H	54	SER
2	H	79	PHE
2	H	85	GLU
2	H	92	CYS
2	H	98	ASP
2	H	101	ASN
2	H	107	THR
2	H	108	MET
2	H	110	THR
2	H	134	THR
2	H	137	THR
2	H	139	THR
2	H	143	LEU
2	H	167	THR
2	H	168	SER
2	H	177	VAL
2	H	188	SER
2	H	192	THR
2	H	193	VAL
2	H	196	SER
2	H	203	SER
2	H	209	ASN
2	H	222	LYS
2	H	223	ILE
3	E	1	ASP
3	E	5	ASN
3	E	11	SER
3	E	19	LEU
3	E	21	CYS
3	E	25	SER
3	E	26	ASP
3	E	34	ASN
3	E	37	GLU

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Mol	Chain	Res	Type
3	E	53	GLU
3	E	54	VAL
3	E	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	52	ASN
1	L	89	GLN
1	L	138	ASN
2	H	76	ASN
2	H	101	ASN
2	H	105	GLN
2	H	204	GLN
3	E	70	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 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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	213/213 (100%)	0.08	1 (0%) 91 88	131, 169, 223, 232	0
2	H	216/216 (100%)	0.07	2 (0%) 85 79	151, 182, 213, 238	0
3	E	82/82 (100%)	0.17	1 (1%) 81 73	166, 180, 190, 215	0
All	All	511/511 (100%)	0.09	4 (0%) 87 82	131, 180, 221, 238	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1	ASP	3.1
1	L	155	LYS	2.6
2	H	24	ALA	2.5
2	H	26	GLY	2.1

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.