



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QR1
Title : POOR BINDING OF A HER-2/NEU EPITOPE (GP2) TO HLA-A2.1 IS
DUE TO A LACK OF INTERACTIONS IN THE CENTER OF THE PEP-
TIDE
Authors : Kuhns, J. J.; Batalia, M. A.; Yan, S.; Collins, E. J.
Deposited on : 1999-06-17
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

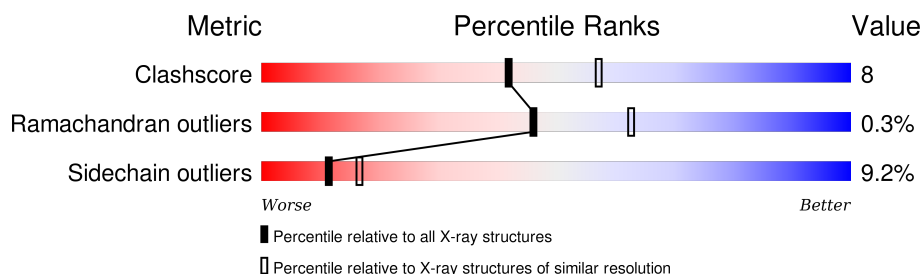
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	
1	D	275	
2	B	100	
2	E	100	
3	C	9	
3	F	9	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6395 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 HLA-A2.1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	ALA	engineered	UNP P61769
E	0	MET	ALA	engineered	UNP P61769

- Molecule 3 is a protein called GP2 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	12	0	0
			62	42	9	11			
3	F	9	Total	C	N	O	11	0	0
			62	42	9	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		

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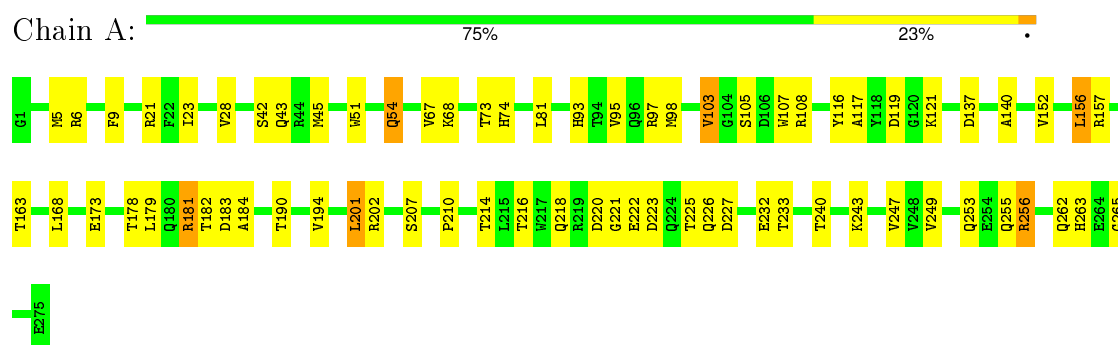
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total 22	O 22	0	0
4	C	1	Total 1	O 1	0	0
4	D	25	Total 25	O 25	0	0
4	E	12	Total 12	O 12	0	0
4	F	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

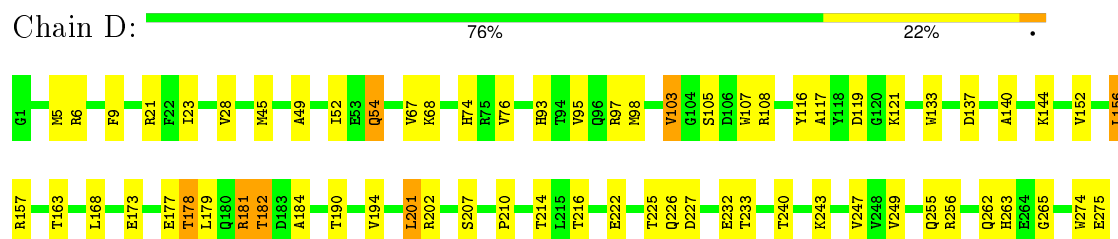
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

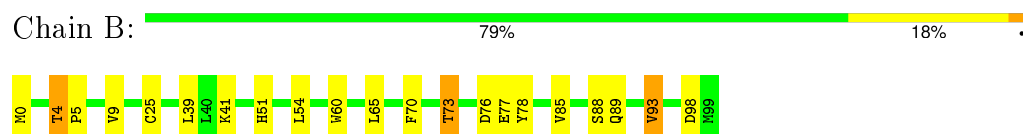
• Molecule 1: HLA-A2.1 HEAVY CHAIN



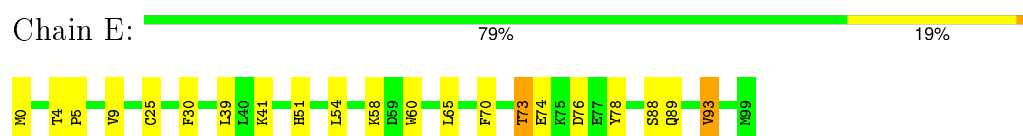
• Molecule 1: HLA-A2.1 HEAVY CHAIN



• Molecule 2: BETA-2 MICROGLOBULIN



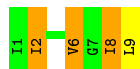
• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 3: GP2 PEPTIDE



- Molecule 3: GP2 PEPTIDE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.34Å 63.61Å 75.14Å 81.88° 76.25° 77.83°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	98.2 (30.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.242 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6395	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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	0.47	1/2312 (0.0%)	0.70	0/3137
1	D	0.45	0/2312	0.71	0/3137
2	B	0.46	0/860	0.70	0/1162
2	E	0.47	0/860	0.70	0/1162
3	C	0.54	0/61	0.88	0/81
3	F	0.67	0/61	0.86	0/81
All	All	0.47	1/6466 (0.0%)	0.71	0/8760

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	THR	CB-CG2	-5.70	1.33	1.52

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	2247	0	2096	42	1
1	D	2247	0	2096	36	1
2	B	837	0	803	12	0
2	E	837	0	803	10	0
3	C	62	0	77	7	0
3	F	62	0	77	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	0	2	0
4	B	22	0	0	3	0
4	C	1	0	0	0	0
4	D	25	0	0	0	0
4	E	12	0	0	0	0
4	F	1	0	0	1	0
All	All	6395	0	5952	101	1

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 8.

All (101) 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:73:THR:HG23	3:C:8:ILE:HD13	1.32	1.05
2:E:73:THR:HG22	2:E:76:ASP:H	1.35	0.91
2:B:73:THR:HG22	2:B:76:ASP:H	1.33	0.90
1:A:73:THR:HG23	3:C:8:ILE:CD1	2.12	0.78
1:A:103:VAL:HG13	1:A:107:TRP:HA	1.72	0.70
2:B:98:ASP:HB3	4:B:108:HOH:O	1.91	0.69
3:F:8:ILE:HG23	4:F:90:HOH:O	1.94	0.67
1:A:116:TYR:CE1	3:C:9:LEU:HD11	2.30	0.66
1:D:263:HIS:CD2	1:D:265:GLY:H	2.14	0.65
2:B:85:VAL:HG13	4:B:104:HOH:O	1.97	0.65
1:A:263:HIS:CD2	1:A:265:GLY:H	2.13	0.65
1:A:218:GLN:NE2	1:A:221:GLY:HA2	2.12	0.65
1:D:233:THR:OG1	1:D:243:LYS:HE3	1.99	0.63
1:D:103:VAL:HG13	1:D:107:TRP:HA	1.81	0.63
1:A:103:VAL:CG1	1:A:107:TRP:HA	2.29	0.62
1:D:116:TYR:CE1	3:F:9:LEU:HD11	2.35	0.62
1:D:178:THR:HG22	1:D:179:LEU:N	2.13	0.61
1:A:233:THR:OG1	1:A:243:LYS:HE3	2.00	0.61
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.30	0.61
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.65	0.61
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.84	0.61
2:E:9:VAL:CG2	2:E:93:VAL:HG22	2.31	0.60
1:D:54:GLN:O	1:D:54:GLN:HG2	2.01	0.59
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.86	0.59
1:D:274:TRP:O	1:D:275:GLU:HB3	2.04	0.57
1:A:54:GLN:O	1:A:54:GLN:HG2	2.04	0.56
2:B:77:GLU:HG2	4:B:107:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.90	0.54
1:A:137:ASP:HB3	1:A:140:ALA:H	1.74	0.53
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.89	0.53
1:D:181:ARG:HD2	1:D:182:THR:H	1.74	0.53
1:D:116:TYR:CZ	3:F:9:LEU:HD11	2.44	0.53
1:D:137:ASP:HB3	1:D:140:ALA:H	1.74	0.53
1:D:103:VAL:CG1	1:D:107:TRP:HA	2.39	0.52
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.91	0.52
2:B:51:HIS:HA	2:B:65:LEU:O	2.10	0.52
1:A:214:THR:HB	1:A:262:GLN:HB2	1.92	0.52
1:D:214:THR:HB	1:D:262:GLN:HB2	1.92	0.51
2:E:51:HIS:HA	2:E:65:LEU:O	2.12	0.50
1:D:152:VAL:HG12	1:D:156:LEU:HD22	1.94	0.50
2:E:9:VAL:HG23	2:E:93:VAL:HG22	1.93	0.50
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.94	0.49
1:A:116:TYR:CZ	3:C:9:LEU:HD11	2.47	0.49
1:A:152:VAL:HG12	1:A:156:LEU:HD22	1.94	0.49
1:A:223:ASP:HB2	4:A:308:HOH:O	2.13	0.49
1:D:263:HIS:HD2	1:D:265:GLY:H	1.59	0.49
1:A:45:MET:HE2	1:A:67:VAL:HB	1.96	0.48
1:A:207:SER:HA	1:A:240:THR:HB	1.96	0.48
1:D:9:PHE:HZ	3:F:2:ILE:CD1	2.27	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.48
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.96	0.47
1:A:263:HIS:HD2	1:A:265:GLY:H	1.58	0.47
1:D:133:TRP:HB2	1:D:144:LYS:HD2	1.96	0.47
1:D:184:ALA:HB2	1:D:265:GLY:O	2.15	0.47
2:B:9:VAL:HG21	2:B:93:VAL:HG22	1.97	0.47
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.96	0.47
1:A:227:ASP:O	1:A:247:VAL:HG12	2.15	0.47
1:D:182:THR:HG21	1:D:265:GLY:HA2	1.96	0.47
2:E:9:VAL:HG21	2:E:93:VAL:HG22	1.96	0.47
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.98	0.46
1:D:227:ASP:O	1:D:247:VAL:HG12	2.15	0.46
1:A:182:THR:HG22	1:A:182:THR:O	2.13	0.46
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.34	0.46
1:A:6:ARG:HD3	1:A:98:MET:HE2	1.98	0.46
1:D:201:LEU:HD23	1:D:249:VAL:HG21	1.96	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.51	0.46
1:A:181:ARG:NE	1:A:183:ASP:OD1	2.46	0.46
1:A:201:LEU:HD23	1:A:249:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:VAL:HG11	1:D:179:LEU:HD13	1.96	0.46
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.16	0.46
1:D:207:SER:HA	1:D:240:THR:HB	1.98	0.45
1:A:184:ALA:HB2	1:A:265:GLY:O	2.16	0.45
1:D:9:PHE:HZ	3:F:2:ILE:HD12	1.81	0.45
2:B:4:THR:HA	2:B:5:PRO:HD3	1.74	0.45
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.35	0.45
1:D:76:VAL:HB	3:F:8:ILE:HD11	1.98	0.45
1:D:210:PRO:O	1:D:263:HIS:HE1	2.00	0.45
1:D:45:MET:CE	1:D:67:VAL:HB	2.47	0.45
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.17	0.44
1:A:81:LEU:HD11	3:C:9:LEU:CD1	2.47	0.44
1:A:210:PRO:O	1:A:263:HIS:HE1	2.00	0.44
1:D:21:ARG:HE	1:D:23:ILE:HD11	1.83	0.44
1:A:220:ASP:OD1	1:A:256:ARG:HB2	2.17	0.44
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.83	0.44
1:A:223:ASP:CB	4:A:308:HOH:O	2.65	0.43
3:C:2:ILE:HA	3:C:2:ILE:HD13	1.81	0.43
1:A:45:MET:CE	1:A:67:VAL:HB	2.48	0.43
2:E:41:LYS:HE3	2:E:78:TYR:OH	2.18	0.43
1:A:9:PHE:HZ	3:C:2:ILE:HD12	1.83	0.42
1:A:182:THR:HG21	1:A:265:GLY:HA2	2.02	0.42
1:D:6:ARG:HD3	1:D:98:MET:HE2	2.01	0.42
1:D:49:ALA:O	1:D:52:ILE:HG22	2.20	0.42
2:E:73:THR:HG23	2:E:74:GLU:N	2.36	0.41
1:A:95:VAL:HG13	1:A:116:TYR:CE1	2.56	0.41
1:A:253:GLN:O	1:A:256:ARG:HG2	2.20	0.41
1:A:42:SER:O	1:A:43:GLN:HB2	2.21	0.41
2:B:41:LYS:HE3	2:B:78:TYR:OH	2.20	0.40
1:D:177:GLU:O	1:D:181:ARG:HB2	2.20	0.40
1:D:95:VAL:HG13	1:D:116:TYR:CE1	2.55	0.40
3:F:2:ILE:HD13	3:F:2:ILE:HA	1.80	0.40
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH1	1:D:182:THR:O[1_454]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
1	D	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	F	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
All	All	756/768 (98%)	739 (98%)	15 (2%)	2 (0%)	46	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	VAL
3	F	6	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	231/231 (100%)	212 (92%)	19 (8%)	14	21
1	D	231/231 (100%)	209 (90%)	22 (10%)	11	15
2	B	95/95 (100%)	87 (92%)	8 (8%)	14	20
2	E	95/95 (100%)	86 (90%)	9 (10%)	11	15
3	C	7/7 (100%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	7/7 (100%)	4 (57%)	3 (43%)	0	0
All	All	666/666 (100%)	605 (91%)	61 (9%)	11	16

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	68	LYS
1	A	103	VAL
1	A	105	SER
1	A	121	LYS
1	A	156	LEU
1	A	157	ARG
1	A	163	THR
1	A	173	GLU
1	A	181	ARG
1	A	194	VAL
1	A	201	LEU
1	A	216	THR
1	A	222	GLU
1	A	225	THR
1	A	226	GLN
1	A	232	GLU
1	A	255	GLN
1	A	256	ARG
2	B	0	MET
2	B	4	THR
2	B	54	LEU
2	B	70	PHE
2	B	73	THR
2	B	88	SER
2	B	89	GLN
2	B	93	VAL
1	D	54	GLN
1	D	68	LYS
1	D	103	VAL
1	D	105	SER
1	D	108	ARG
1	D	121	LYS
1	D	156	LEU
1	D	157	ARG
1	D	163	THR

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Mol	Chain	Res	Type
1	D	173	GLU
1	D	178	THR
1	D	181	ARG
1	D	182	THR
1	D	194	VAL
1	D	201	LEU
1	D	216	THR
1	D	222	GLU
1	D	225	THR
1	D	226	GLN
1	D	232	GLU
1	D	255	GLN
1	D	256	ARG
2	E	0	MET
2	E	4	THR
2	E	54	LEU
2	E	58	LYS
2	E	70	PHE
2	E	73	THR
2	E	88	SER
2	E	89	GLN
2	E	93	VAL
3	F	2	ILE
3	F	6	VAL
3	F	8	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	93	HIS
1	A	96	GLN
1	A	114	HIS
1	A	218	GLN
1	A	263	HIS
1	D	54	GLN
1	D	93	HIS
1	D	96	GLN
1	D	114	HIS
1	D	218	GLN
1	D	263	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.