Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:57 PM GMT

PDB ID	:	5F6J
Title	:	Crystal Structure of Tier 2 Neutralizing Antibody DH427 from a Rhesus Macaque in Complex with HIV-1 gp120 Core
Authors	:	Fera, D.; Harrison, S.C.
Deposited on	:	2015-12-06
Resolution	:	6.63 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:

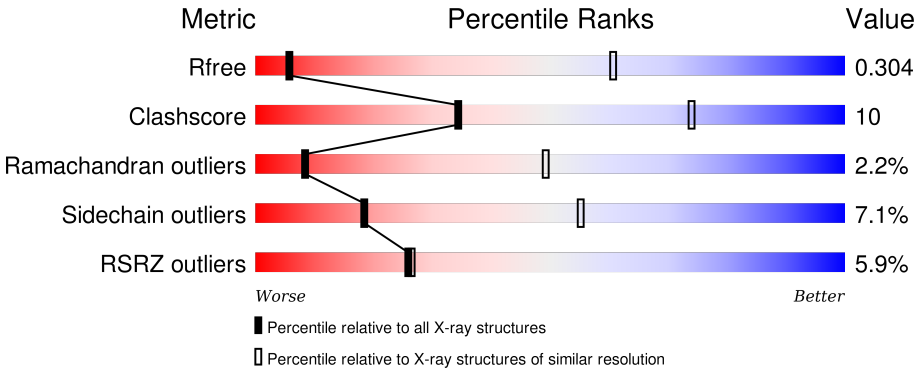
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 6.63 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.



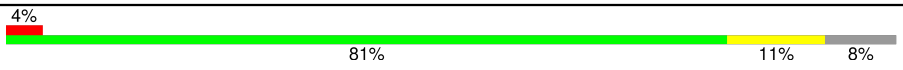
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 <=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	E	352	8% 63% 27% 6% • 5%
1	G	352	9% 63% 27% 5% • 5%
2	A	216	4% 87% 11% •
2	F	216	5% 88% 9% • •
3	B	228	2% 81% 11% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	228	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11572 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 ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	336	Total	C	N	O	S	0	0	0
			2640	1659	458	502	21			
1	E	336	Total	C	N	O	S	0	0	0
			2640	1659	458	502	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	458	LYS	GLY	engineered mutation	UNP R4GRV3
G	?	-	GLY	deletion	UNP R4GRV3
G	?	-	ASN	deletion	UNP R4GRV3
G	?	-	ASP	deletion	UNP R4GRV3
G	463	SER	ASN	engineered mutation	UNP R4GRV3
G	464	ASN	ASP	engineered mutation	UNP R4GRV3
E	458	LYS	GLY	engineered mutation	UNP R4GRV3
E	?	-	GLY	deletion	UNP R4GRV3
E	?	-	ASN	deletion	UNP R4GRV3
E	?	-	ASP	deletion	UNP R4GRV3
E	463	SER	ASN	engineered mutation	UNP R4GRV3
E	464	ASN	ASP	engineered mutation	UNP R4GRV3

- Molecule 2 is a protein called DH427 Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			
2	F	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			

- Molecule 3 is a protein called DH427 Antibody Heavy Chain.

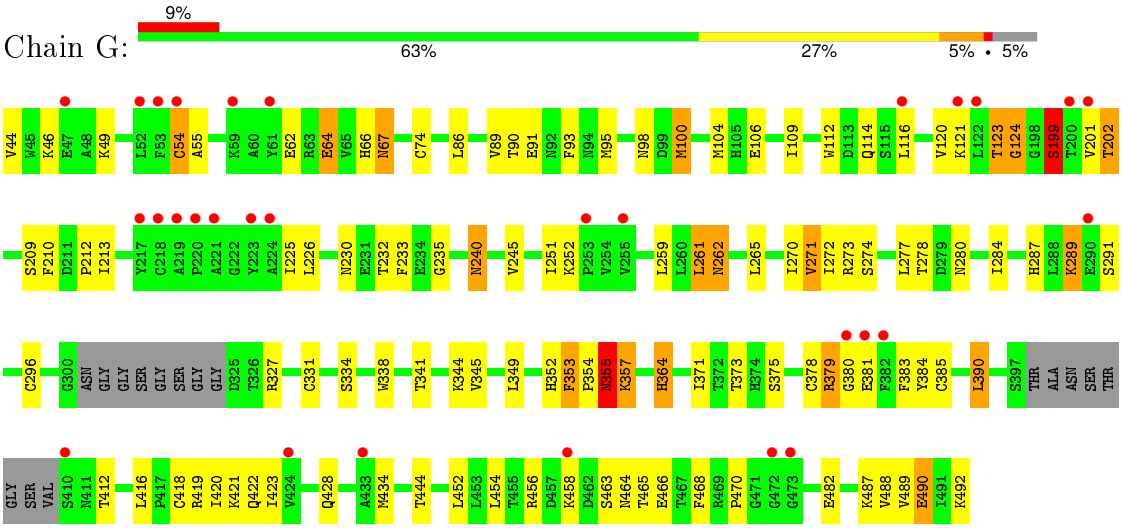
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			
3	H	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			

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 (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.

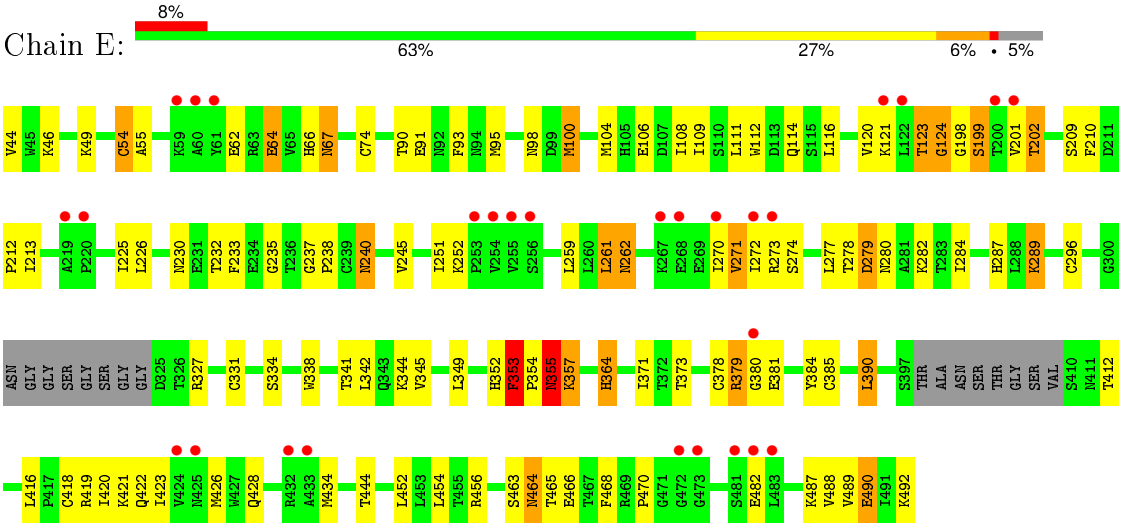
- Molecule 1: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C

Chain G:



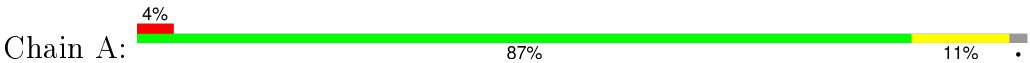
- Molecule 1: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C

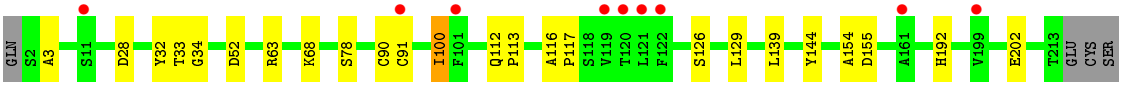
Chain E:



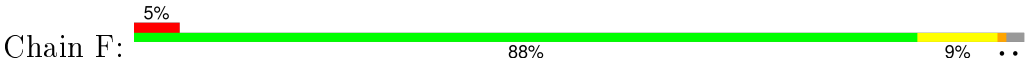
- Molecule 2: DH427 Antibody Light Chain

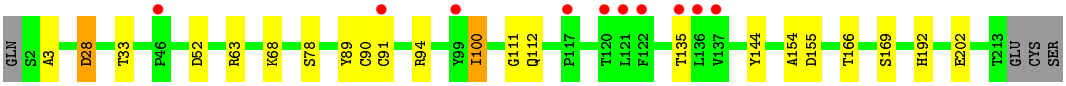
Chain A:



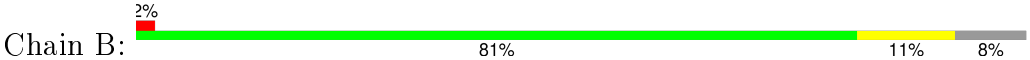


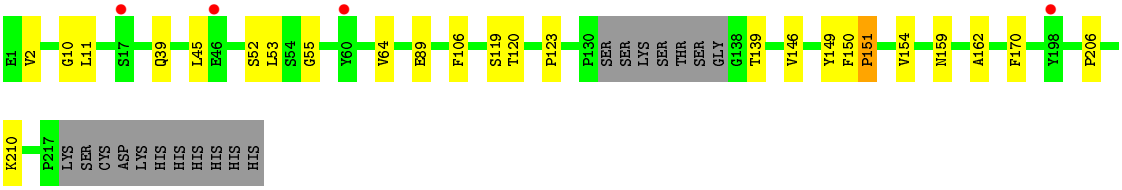
• Molecule 2: DH427 Antibody Light Chain



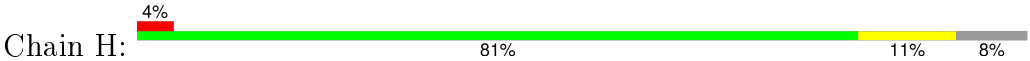


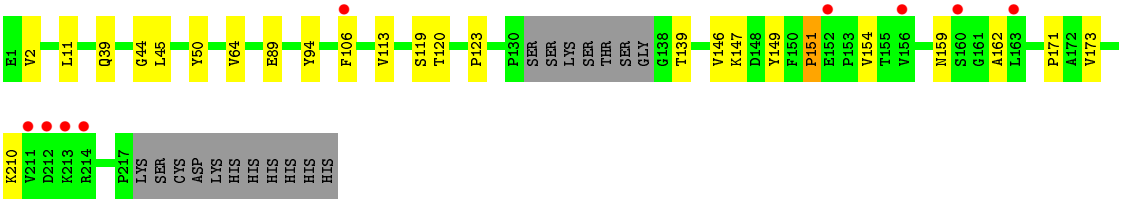
• Molecule 3: DH427 Antibody Heavy Chain





• Molecule 3: DH427 Antibody Heavy Chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	162.90Å 162.90Å 229.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	141.08 – 6.63 141.08 – 6.63	Depositor EDS
% Data completeness (in resolution range)	93.2 (141.08-6.63) 93.2 (141.08-6.63)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 6.73Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.256 , 0.305 0.257 , 0.304	Depositor DCC
R_{free} test set	301 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	306.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 254.1	EDS
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 6058 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11572	wwPDB-VP
Average B, all atoms (Å^2)	276.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	E	0.46	0/2697	0.73	2/3658 (0.1%)
1	G	0.46	0/2697	0.72	1/3658 (0.0%)
2	A	0.46	0/1610	0.62	0/2198
2	F	0.47	0/1610	0.63	0/2198
3	B	0.47	0/1610	0.66	0/2193
3	H	0.48	0/1610	0.66	0/2193
All	All	0.47	0/11834	0.68	3/16098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	261	LEU	CA-CB-CG	6.66	130.61	115.30
1	E	261	LEU	CA-CB-CG	6.64	130.56	115.30
1	E	353	PHE	C-N-CD	-5.17	109.23	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	E	2640	0	2592	85	0
1	G	2640	0	2592	106	0
2	A	1574	0	1525	42	0
2	F	1574	0	1525	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1572	0	1530	10	0
3	H	1572	0	1530	12	0
All	All	11572	0	11294	229	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 10.

All (229) 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:G:357:LYS:HE3	1:G:466:GLU:CG	1.17	1.65
1:G:357:LYS:CE	1:G:466:GLU:HG3	1.21	1.62
1:G:355:ASN:OD1	2:A:33:THR:C	1.75	1.25
1:G:355:ASN:O	1:G:357:LYS:HG3	1.08	1.25
1:G:357:LYS:O	2:A:32:TYR:CE1	1.90	1.25
1:G:357:LYS:O	2:A:32:TYR:HE1	1.14	1.23
1:E:355:ASN:O	1:E:357:LYS:HG3	1.39	1.19
1:G:357:LYS:C	2:A:32:TYR:HE1	1.46	1.18
1:G:355:ASN:CB	2:A:33:THR:H	1.58	1.16
1:E:353:PHE:CD2	1:E:354:PRO:HD2	1.80	1.14
1:G:355:ASN:O	1:G:357:LYS:CG	1.96	1.13
1:G:357:LYS:HE3	1:G:466:GLU:HG2	1.23	1.09
1:G:357:LYS:NZ	1:G:466:GLU:HG3	1.67	1.07
1:G:355:ASN:HB3	2:A:33:THR:H	1.07	1.07
1:E:353:PHE:HD2	1:E:354:PRO:HD2	0.91	1.07
1:G:355:ASN:HB3	2:A:33:THR:N	1.72	1.04
1:E:355:ASN:O	1:E:357:LYS:CG	2.06	1.04
1:G:123:THR:O	1:G:199:SER:OG	1.79	1.00
1:E:354:PRO:O	1:E:355:ASN:ND2	1.98	0.97
1:G:357:LYS:C	2:A:32:TYR:CE1	2.37	0.96
1:E:123:THR:O	1:E:124:GLY:O	1.86	0.93
1:G:357:LYS:HB3	1:G:466:GLU:HG2	1.48	0.93
1:G:355:ASN:OD1	2:A:34:GLY:N	2.03	0.92
1:G:354:PRO:O	1:G:355:ASN:ND2	2.05	0.90
1:G:355:ASN:OD1	2:A:33:THR:CA	2.22	0.88
1:E:357:LYS:NZ	1:E:466:GLU:HG3	1.90	0.85
1:G:357:LYS:N	2:A:32:TYR:HD1	1.74	0.84
1:G:357:LYS:N	2:A:32:TYR:CD1	2.48	0.81
1:E:355:ASN:O	1:E:357:LYS:CB	2.31	0.78
1:G:458:LYS:O	3:B:53:LEU:HD21	1.84	0.78
1:G:357:LYS:CE	1:G:466:GLU:CG	2.04	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:HG	1:E:487:LYS:HB2	1.65	0.78
3:B:123:PRO:HB3	3:B:149:TYR:HB3	1.67	0.76
1:G:226:LEU:HG	1:G:487:LYS:HB2	1.67	0.75
1:G:419:ARG:HH12	1:G:421:LYS:HE2	1.51	0.74
1:G:357:LYS:CA	2:A:32:TYR:CE1	2.70	0.74
3:H:123:PRO:HB3	3:H:149:TYR:HB3	1.70	0.73
1:E:419:ARG:HH12	1:E:421:LYS:HE2	1.54	0.73
1:E:355:ASN:HB3	2:F:33:THR:H	1.54	0.72
1:E:357:LYS:HB3	1:E:466:GLU:HG2	1.72	0.71
1:E:120:VAL:HG23	1:E:202:THR:HB	1.72	0.71
1:G:355:ASN:CG	2:A:33:THR:H	1.95	0.70
1:E:355:ASN:C	1:E:357:LYS:HG3	2.09	0.70
1:E:353:PHE:CG	1:E:357:LYS:HD2	2.27	0.69
1:G:357:LYS:H	2:A:32:TYR:HD1	1.40	0.69
1:E:355:ASN:OD1	2:F:33:THR:OG1	2.03	0.69
1:G:357:LYS:CA	2:A:32:TYR:HE1	2.03	0.69
1:G:120:VAL:HG23	1:G:202:THR:HB	1.75	0.68
1:E:357:LYS:HE3	1:E:466:GLU:CG	2.26	0.64
1:E:124:GLY:O	1:E:199:SER:N	2.30	0.64
1:G:355:ASN:CB	2:A:33:THR:N	2.41	0.63
1:E:230:ASN:HB3	1:E:233:PHE:HB2	1.80	0.63
1:G:355:ASN:C	1:G:357:LYS:HG3	2.10	0.63
1:E:252:LYS:HE3	1:E:262:ASN:HB3	1.80	0.63
1:G:212:PRO:HB2	1:G:252:LYS:HD2	1.80	0.63
1:G:357:LYS:HB3	1:G:466:GLU:CG	2.24	0.62
1:G:230:ASN:HB3	1:G:233:PHE:HB2	1.82	0.62
1:E:251:ILE:HG12	1:E:482:GLU:HG3	1.81	0.62
1:E:123:THR:O	1:E:124:GLY:C	2.38	0.62
1:G:252:LYS:HE3	1:G:262:ASN:HB3	1.81	0.61
3:H:159:ASN:HB2	3:H:162:ALA:HB3	1.82	0.61
2:F:166:THR:HG22	3:H:173:VAL:HA	1.82	0.61
1:G:251:ILE:HG12	1:G:482:GLU:HG3	1.83	0.61
1:G:355:ASN:HB2	2:A:32:TYR:HB3	1.81	0.61
1:G:355:ASN:HB3	2:A:32:TYR:HA	1.84	0.60
1:E:98:ASN:HB3	1:E:100:MET:HG2	1.84	0.60
1:G:355:ASN:OD1	2:A:33:THR:OG1	2.21	0.58
1:E:373:THR:HG21	1:E:384:TYR:HD2	1.68	0.58
1:E:357:LYS:HZ2	1:E:466:GLU:HG3	1.69	0.58
1:G:355:ASN:OD1	2:A:33:THR:N	2.35	0.58
1:G:373:THR:HG21	1:G:384:TYR:HD2	1.68	0.57
1:E:422:GLN:HB3	1:E:434:MET:SD	2.44	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LYS:CE	1:E:466:GLU:HG3	2.34	0.57
1:G:355:ASN:CB	2:A:32:TYR:HA	2.35	0.56
1:E:95:MET:HG3	1:E:235:GLY:HA2	1.86	0.56
1:G:225:ILE:HG13	1:G:245:VAL:HG13	1.88	0.56
1:G:98:ASN:HB3	1:G:100:MET:HG2	1.86	0.56
1:E:212:PRO:HB2	1:E:252:LYS:HD2	1.88	0.56
1:E:355:ASN:O	1:E:357:LYS:HB2	2.06	0.55
1:E:421:LYS:HD2	1:E:423:ILE:HG13	1.86	0.55
2:A:33:THR:HG22	2:A:68:LYS:HE2	1.87	0.55
1:G:95:MET:HG3	1:G:235:GLY:HA2	1.87	0.55
1:E:225:ILE:HG13	1:E:245:VAL:HG13	1.88	0.55
1:G:357:LYS:O	2:A:32:TYR:CZ	2.58	0.55
1:E:353:PHE:CD2	1:E:354:PRO:CD	2.72	0.55
1:G:106:GLU:HA	1:G:109:ILE:HD12	1.89	0.55
1:E:353:PHE:HB3	1:E:357:LYS:HD3	1.89	0.55
1:G:421:LYS:HD2	1:G:423:ILE:HG13	1.87	0.55
1:G:95:MET:HE1	1:G:487:LYS:HE3	1.89	0.54
3:B:11:LEU:HD13	3:B:151:PRO:HG3	1.88	0.54
1:G:352:HIS:CG	1:G:353:PHE:N	2.75	0.54
2:A:113:PRO:HB3	2:F:111:GLY:O	2.07	0.54
2:F:63:ARG:HB3	2:F:78:SER:O	2.08	0.54
1:E:352:HIS:CG	1:E:353:PHE:N	2.76	0.54
1:E:106:GLU:HA	1:E:109:ILE:HD12	1.90	0.54
1:E:341:THR:O	1:E:344:LYS:HG2	2.07	0.54
1:E:357:LYS:HE3	1:E:466:GLU:HG2	1.90	0.53
1:E:364:HIS:HD2	1:E:470:PRO:HG2	1.74	0.53
2:A:154:ALA:HB1	2:A:192:HIS:CD2	2.44	0.53
1:G:422:GLN:HB3	1:G:434:MET:SD	2.49	0.52
1:E:357:LYS:HZ1	1:E:466:GLU:HG3	1.71	0.52
1:E:54:CYS:SG	1:E:55:ALA:N	2.83	0.52
1:G:364:HIS:HD2	1:G:470:PRO:HG2	1.75	0.51
1:E:284:ILE:HD11	1:E:454:LEU:HB2	1.93	0.51
1:E:355:ASN:CB	2:F:33:THR:H	2.20	0.51
3:H:11:LEU:HD13	3:H:151:PRO:HG3	1.92	0.51
1:E:353:PHE:HB3	1:E:357:LYS:CD	2.40	0.50
1:G:54:CYS:SG	1:G:55:ALA:N	2.85	0.50
2:F:112:GLN:HB2	2:F:144:TYR:CZ	2.46	0.50
2:F:89:TYR:CE2	3:H:44:GLY:HA2	2.47	0.50
1:E:463:SER:C	1:E:465:THR:H	2.15	0.50
1:G:454:LEU:HD23	1:G:470:PRO:HA	1.94	0.50
1:G:341:THR:O	1:G:344:LYS:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:357:LYS:HA	2:A:32:TYR:CE1	2.47	0.49
2:F:33:THR:HG22	2:F:68:LYS:HE2	1.93	0.49
1:G:284:ILE:HD11	1:G:454:LEU:HB2	1.93	0.49
2:F:3:ALA:HA	2:F:100:ILE:HD11	1.94	0.49
2:F:154:ALA:HB1	2:F:192:HIS:CD2	2.47	0.49
1:E:62:GLU:OE1	1:E:67:ASN:ND2	2.45	0.49
1:E:454:LEU:HD23	1:E:470:PRO:HA	1.95	0.49
3:H:146:VAL:HG11	3:H:154:VAL:HG11	1.93	0.49
1:G:355:ASN:HB3	2:A:32:TYR:CA	2.41	0.49
1:G:62:GLU:OE1	1:G:67:ASN:ND2	2.46	0.49
2:A:112:GLN:HB2	2:A:144:TYR:CZ	2.48	0.49
1:E:271:VAL:HG22	1:E:287:HIS:HE2	1.78	0.49
3:B:159:ASN:HB2	3:B:162:ALA:HB3	1.94	0.49
1:G:463:SER:C	1:G:465:THR:H	2.16	0.49
1:G:270:ILE:H	1:G:270:ILE:HD12	1.78	0.49
1:G:357:LYS:NZ	1:G:466:GLU:CG	2.57	0.48
2:A:63:ARG:HB3	2:A:78:SER:O	2.13	0.48
1:G:354:PRO:C	1:G:355:ASN:ND2	2.66	0.48
1:E:95:MET:HE1	1:E:487:LYS:HE3	1.95	0.48
1:G:123:THR:O	1:G:124:GLY:C	2.52	0.48
1:G:124:GLY:O	1:G:199:SER:OG	2.32	0.48
1:G:64:GLU:HG2	1:G:67:ASN:HD21	1.78	0.48
3:B:39:GLN:HB2	3:B:45:LEU:HD23	1.96	0.48
1:G:64:GLU:HB2	1:G:209:SER:O	2.14	0.47
3:B:146:VAL:HG11	3:B:154:VAL:HG11	1.95	0.47
1:E:64:GLU:HG2	1:E:67:ASN:HD21	1.79	0.47
1:E:271:VAL:HG22	1:E:287:HIS:NE2	2.29	0.47
1:G:44:VAL:HG11	1:G:492:LYS:H	1.79	0.47
1:E:64:GLU:HB2	1:E:209:SER:O	2.14	0.47
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.97	0.47
1:E:355:ASN:HB3	2:F:33:THR:N	2.27	0.47
1:E:270:ILE:H	1:E:270:ILE:HD12	1.80	0.47
2:A:33:THR:O	2:A:52:ASP:HA	2.15	0.47
1:G:355:ASN:HB2	2:A:32:TYR:CB	2.45	0.47
1:G:357:LYS:N	2:A:32:TYR:CE1	2.83	0.47
1:E:364:HIS:CD2	1:E:470:PRO:HG2	2.49	0.47
1:G:364:HIS:CD2	1:G:470:PRO:HG2	2.50	0.47
1:G:271:VAL:HG22	1:G:287:HIS:NE2	2.30	0.47
1:E:46:LYS:HB3	1:E:490:GLU:HB2	1.97	0.47
3:B:150:PHE:HA	3:B:151:PRO:HA	1.75	0.46
1:E:464:ASN:HB2	3:H:50:TYR:CZ	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:ARG:HH12	1:G:421:LYS:CE	2.26	0.46
1:E:270:ILE:HG13	1:E:289:LYS:HB2	1.98	0.46
1:G:345:VAL:O	1:G:349:LEU:HG	2.14	0.46
1:G:327:ARG:HD3	1:G:420:ILE:HG13	1.98	0.45
1:G:90:THR:HG22	1:G:240:ASN:HA	1.97	0.45
1:G:46:LYS:HB3	1:G:490:GLU:HB2	1.97	0.45
1:E:373:THR:HG21	1:E:384:TYR:CD2	2.51	0.45
1:G:271:VAL:HG22	1:G:287:HIS:HE2	1.81	0.45
1:E:210:PHE:O	1:E:379:ARG:HG3	2.16	0.45
1:E:112:TRP:HE3	1:E:428:GLN:HE22	1.65	0.45
1:G:338:TRP:CZ2	1:G:390:LEU:HB2	2.51	0.45
3:H:159:ASN:CB	3:H:162:ALA:HB3	2.47	0.45
1:E:456:ARG:HD2	1:E:468:PHE:CE1	2.52	0.45
1:G:456:ARG:HD2	1:G:468:PHE:CE1	2.52	0.45
1:G:270:ILE:HG13	1:G:289:LYS:HB2	1.99	0.44
2:F:33:THR:O	2:F:52:ASP:HA	2.16	0.44
1:G:123:THR:O	1:G:124:GLY:O	2.35	0.44
1:E:327:ARG:HD3	1:E:420:ILE:HG13	1.99	0.44
1:E:44:VAL:HG11	1:E:492:LYS:H	1.82	0.44
1:G:355:ASN:HB3	2:A:32:TYR:C	2.34	0.44
1:G:373:THR:HG21	1:G:384:TYR:CD2	2.50	0.44
1:G:259:LEU:HD23	1:G:452:LEU:HD13	2.00	0.44
1:G:265:LEU:HD21	1:G:291:SER:HB3	2.00	0.44
3:B:10:GLY:HA2	3:B:206:PRO:HG3	2.00	0.43
1:G:210:PHE:O	1:G:379:ARG:HG3	2.18	0.43
2:A:126:SER:HA	2:A:129:LEU:HD12	2.00	0.43
1:E:90:THR:HG22	1:E:240:ASN:HA	1.99	0.43
1:E:364:HIS:HE1	1:E:371:ILE:HD12	1.83	0.43
1:E:93:PHE:HE2	1:E:98:ASN:HD21	1.66	0.43
1:G:93:PHE:HE2	1:G:98:ASN:HD21	1.65	0.43
1:G:456:ARG:HD2	1:G:468:PHE:HE1	1.82	0.43
2:F:169:SER:OG	3:H:171:PRO:HG2	2.19	0.43
1:G:355:ASN:CB	2:A:32:TYR:CA	2.95	0.43
2:A:112:GLN:HB2	2:A:144:TYR:CE2	2.54	0.43
1:E:419:ARG:HH12	1:E:421:LYS:CE	2.27	0.42
1:E:342:LEU:HA	1:E:345:VAL:HB	2.01	0.42
1:E:259:LEU:HD23	1:E:452:LEU:HD13	2.01	0.42
1:E:385:CYS:HA	1:E:418:CYS:HA	2.02	0.42
1:G:109:ILE:HG23	1:G:428:GLN:HG2	2.01	0.42
1:G:364:HIS:HE1	1:G:371:ILE:HD12	1.84	0.42
1:E:338:TRP:CZ2	1:E:390:LEU:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:LEU:HD23	1:E:416:LEU:HD21	2.00	0.42
2:A:139:LEU:HB3	3:B:170:PHE:CZ	2.54	0.42
1:G:120:VAL:HG12	1:G:434:MET:HB3	2.02	0.42
1:G:375:SER:HA	1:G:383:PHE:O	2.20	0.42
1:E:274:SER:HB2	1:E:284:ILE:HA	2.02	0.42
2:F:135:THR:OG1	3:H:147:LYS:HE3	2.20	0.42
2:A:3:ALA:HA	2:A:100:ILE:HD11	2.01	0.42
1:E:120:VAL:HA	1:E:201:VAL:O	2.20	0.41
1:G:487:LYS:HA	1:G:487:LYS:HD3	1.98	0.41
3:H:94:TYR:CE2	3:H:113:VAL:HB	2.55	0.41
1:E:279:ASP:O	1:E:282:LYS:HG2	2.20	0.41
1:G:64:GLU:HB2	1:G:209:SER:C	2.41	0.41
1:E:456:ARG:HD2	1:E:468:PHE:HE1	1.83	0.41
1:G:378:CYS:O	1:G:379:ARG:HB2	2.20	0.41
1:E:109:ILE:HG23	1:E:428:GLN:HG2	2.02	0.41
2:F:112:GLN:HB2	2:F:144:TYR:CE2	2.55	0.41
1:G:355:ASN:OD1	2:A:33:THR:CB	2.69	0.41
1:E:345:VAL:O	1:E:349:LEU:HG	2.20	0.41
1:G:112:TRP:HE3	1:G:428:GLN:HE22	1.69	0.41
1:E:378:CYS:O	1:E:379:ARG:HB2	2.21	0.41
3:B:52:SER:OG	3:B:55:GLY:O	2.39	0.41
1:G:357:LYS:CA	2:A:32:TYR:CD1	3.01	0.41
1:E:120:VAL:CG2	1:E:202:THR:HB	2.47	0.41
1:G:120:VAL:HA	1:G:201:VAL:O	2.21	0.41
1:G:390:LEU:HD23	1:G:416:LEU:HD21	2.03	0.41
1:G:86:LEU:HB3	1:G:89:VAL:CG1	2.51	0.41
1:G:385:CYS:HA	1:G:418:CYS:HA	2.03	0.41
1:E:237:GLY:HA3	1:E:238:PRO:HD3	1.87	0.41
1:G:274:SER:HB2	1:G:284:ILE:HA	2.03	0.40
2:F:28:ASP:HB3	2:F:94:ARG:HG3	2.03	0.40
2:A:116:ALA:HA	2:A:117:PRO:HD3	1.95	0.40
1:E:352:HIS:CG	1:E:353:PHE:H	2.40	0.40
1:E:108:ILE:HA	1:E:111:LEU:HB3	2.03	0.40
1:E:64:GLU:HB2	1:E:209:SER:C	2.41	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	E	330/352 (94%)	291 (88%)	28 (8%)	11 (3%)	5 40
1	G	330/352 (94%)	290 (88%)	30 (9%)	10 (3%)	5 42
2	A	210/216 (97%)	196 (93%)	12 (6%)	2 (1%)	19 65
2	F	210/216 (97%)	195 (93%)	13 (6%)	2 (1%)	19 65
3	B	206/228 (90%)	189 (92%)	13 (6%)	4 (2%)	10 52
3	H	206/228 (90%)	189 (92%)	13 (6%)	4 (2%)	10 52
All	All	1492/1592 (94%)	1350 (90%)	109 (7%)	33 (2%)	8 49

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	124	GLY
1	G	280	ASN
1	G	355	ASN
1	G	412	THR
1	E	124	GLY
1	E	198	GLY
1	E	280	ASN
1	E	357	LYS
1	E	412	THR
1	E	355	ASN
2	A	202	GLU
3	B	106	PHE
2	F	202	GLU
3	H	106	PHE
1	G	262	ASN
1	G	357	LYS
1	E	199	SER
2	A	155	ASP
3	B	119	SER
2	F	155	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	199	SER
1	G	379	ARG
1	G	464	ASN
1	E	262	ASN
1	E	379	ARG
1	E	464	ASN
3	B	139	THR
3	H	119	SER
3	H	139	THR
1	G	380	GLY
1	E	380	GLY
3	H	151	PRO
3	B	151	PRO

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	E	299/308 (97%)	261 (87%)	38 (13%)	5 29
1	G	299/308 (97%)	262 (88%)	37 (12%)	6 30
2	A	179/183 (98%)	175 (98%)	4 (2%)	60 83
2	F	179/183 (98%)	175 (98%)	4 (2%)	60 83
3	B	175/192 (91%)	170 (97%)	5 (3%)	50 78
3	H	175/192 (91%)	170 (97%)	5 (3%)	50 78
All	All	1306/1366 (96%)	1213 (93%)	93 (7%)	18 55

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	49	LYS
1	G	54	CYS
1	G	64	GLU
1	G	66	HIS
1	G	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	74	CYS
1	G	91	GLU
1	G	100	MET
1	G	104	MET
1	G	114	GLN
1	G	116	LEU
1	G	121	LYS
1	G	123	THR
1	G	199	SER
1	G	202	THR
1	G	213	ILE
1	G	232	THR
1	G	240	ASN
1	G	261	LEU
1	G	271	VAL
1	G	272	ILE
1	G	273	ARG
1	G	277	LEU
1	G	278	THR
1	G	289	LYS
1	G	296	CYS
1	G	331	CYS
1	G	334	SER
1	G	353	PHE
1	G	355	ASN
1	G	364	HIS
1	G	381	GLU
1	G	390	LEU
1	G	444	THR
1	G	488	VAL
1	G	489	VAL
1	G	490	GLU
1	E	49	LYS
1	E	54	CYS
1	E	64	GLU
1	E	66	HIS
1	E	67	ASN
1	E	74	CYS
1	E	91	GLU
1	E	100	MET
1	E	104	MET
1	E	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	116	LEU
1	E	121	LYS
1	E	123	THR
1	E	202	THR
1	E	213	ILE
1	E	232	THR
1	E	240	ASN
1	E	261	LEU
1	E	271	VAL
1	E	272	ILE
1	E	273	ARG
1	E	277	LEU
1	E	278	THR
1	E	279	ASP
1	E	289	LYS
1	E	296	CYS
1	E	331	CYS
1	E	334	SER
1	E	353	PHE
1	E	355	ASN
1	E	364	HIS
1	E	381	GLU
1	E	390	LEU
1	E	426	MET
1	E	444	THR
1	E	488	VAL
1	E	489	VAL
1	E	490	GLU
2	A	28	ASP
2	A	90	CYS
2	A	91	CYS
2	A	100	ILE
3	B	2	VAL
3	B	64	VAL
3	B	89	GLU
3	B	120	THR
3	B	210	LYS
2	F	28	ASP
2	F	90	CYS
2	F	91	CYS
2	F	100	ILE
3	H	2	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	64	VAL
3	H	89	GLU
3	H	120	THR
3	H	210	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	67	ASN
1	G	98	ASN
1	G	103	GLN
1	G	114	GLN
1	G	246	GLN
1	G	332	ASN
1	G	364	HIS
1	E	67	ASN
1	E	98	ASN
1	E	103	GLN
1	E	246	GLN
1	E	332	ASN
1	E	364	HIS
2	A	171	GLN
3	B	175	GLN
2	F	81	GLN
2	F	171	GLN
3	H	57	ASN
3	H	168	HIS
3	H	175	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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^{th} 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	E	336/352 (95%)	0.40	28 (8%)	14	18	156, 278, 397, 462	0
1	G	336/352 (95%)	0.45	30 (8%)	12	16	157, 290, 405, 460	0
2	A	212/216 (98%)	0.12	9 (4%)	40	38	186, 271, 303, 317	0
2	F	212/216 (98%)	0.07	10 (4%)	35	35	144, 272, 309, 322	0
3	B	210/228 (92%)	0.10	4 (1%)	70	65	173, 273, 293, 305	0
3	H	210/228 (92%)	0.33	9 (4%)	39	37	172, 267, 293, 302	0
All	All	1516/1592 (95%)	0.27	90 (5%)	26	26	144, 274, 362, 462	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	472	GLY	8.7
1	E	473	GLY	8.6
1	E	121	LYS	4.9
1	G	219	ALA	4.4
3	H	213	LYS	4.0
3	H	212	ASP	3.9
3	H	214	ARG	3.9
1	E	60	ALA	3.9
1	E	219	ALA	3.8
1	E	253	PRO	3.7
2	A	120	THR	3.6
2	A	119	VAL	3.6
3	H	160	SER	3.4
1	G	200	THR	3.4
1	E	61	TYR	3.4
2	F	122	PHE	3.3
1	G	121	LYS	3.3
1	E	255	VAL	3.3
1	E	482	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	121	LEU	3.2
1	G	220	PRO	3.2
1	G	472	GLY	3.1
1	E	272	ILE	3.1
1	E	432	ARG	3.0
2	F	46	PRO	3.0
1	E	254	VAL	2.9
1	E	433	ALA	2.9
1	G	59	LYS	2.9
1	E	256	SER	2.9
2	F	137	VAL	2.9
1	E	122	LEU	2.9
1	E	200	THR	2.8
1	G	253	PRO	2.8
2	F	117	PRO	2.8
3	H	156	VAL	2.7
1	G	122	LEU	2.7
1	E	481	SER	2.7
1	G	52	LEU	2.6
1	E	220	PRO	2.6
1	E	267	LYS	2.6
1	G	53	PHE	2.6
1	E	273	ARG	2.6
2	F	136	LEU	2.5
1	G	424	VAL	2.5
1	G	218	CYS	2.5
3	H	211	VAL	2.5
1	G	54	CYS	2.5
3	B	17	SER	2.4
1	G	381	GLU	2.4
1	E	425	ASN	2.4
1	E	380	GLY	2.4
1	G	61	TYR	2.4
1	G	255	VAL	2.4
3	B	46	GLU	2.4
2	A	199	VAL	2.4
1	G	223	TYR	2.3
1	G	217	TYR	2.3
1	G	290	GLU	2.3
2	F	135	THR	2.3
2	F	91	CYS	2.3
3	H	163	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	198	TYR	2.3
1	G	433	ALA	2.3
2	A	11	SER	2.3
1	E	424	VAL	2.3
2	A	161	ALA	2.3
1	G	201	VAL	2.3
1	G	380	GLY	2.2
3	H	152	GLU	2.2
1	G	224	ALA	2.2
1	E	270	ILE	2.2
1	E	59	LYS	2.2
3	H	106	PHE	2.2
1	G	47	GLU	2.2
1	G	458	LYS	2.2
2	F	99	TYR	2.2
2	A	122	PHE	2.2
1	G	382	PHE	2.1
1	E	268	GLU	2.1
1	E	483	LEU	2.1
2	A	91	CYS	2.1
2	A	101	PHE	2.1
2	F	120	THR	2.1
1	G	116	LEU	2.1
2	A	121	LEU	2.1
1	E	201	VAL	2.1
1	G	473	GLY	2.0
1	G	221	ALA	2.0
1	G	410	SER	2.0
3	B	60	TYR	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.