



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:17 AM UTC

PDB ID : 3V7A / pdb_00003v7a
Title : Structural basis for broad detection of genogroup II noroviruses by a monoclonal antibody that binds to a site occluded in the viral particle
Authors : Hansman, G.S.; Mclellan, J.S.; Kwong, P.D.
Deposited on : 2011-12-20
Resolution : 3.30 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

<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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

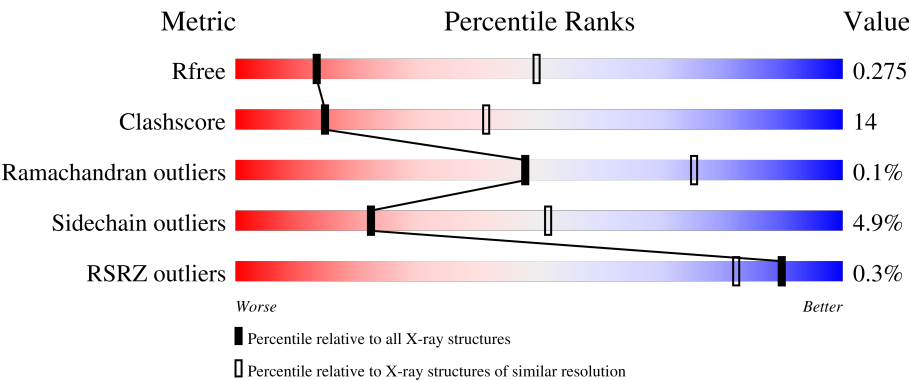
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 ≥ 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	E	223	61%34%..
1	F	223	% 62%33%..
2	G	215	70%29%.
2	H	215	73%26%
3	A	315	70%29%.

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Mol	Chain	Length	Quality of chain
3	B	315	71% 26% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11459 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 5B18 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	220	Total	C	N	O	S	0	0	0
			1643	1035	273	328	7			
1	E	220	Total	C	N	O	S	0	0	0
			1643	1035	273	328	7			

- Molecule 2 is a protein called 5B18 kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	215	Total	C	N	O	S	0	0	0
			1671	1044	281	339	7			
2	H	215	Total	C	N	O	S	0	0	0
			1671	1044	281	339	7			

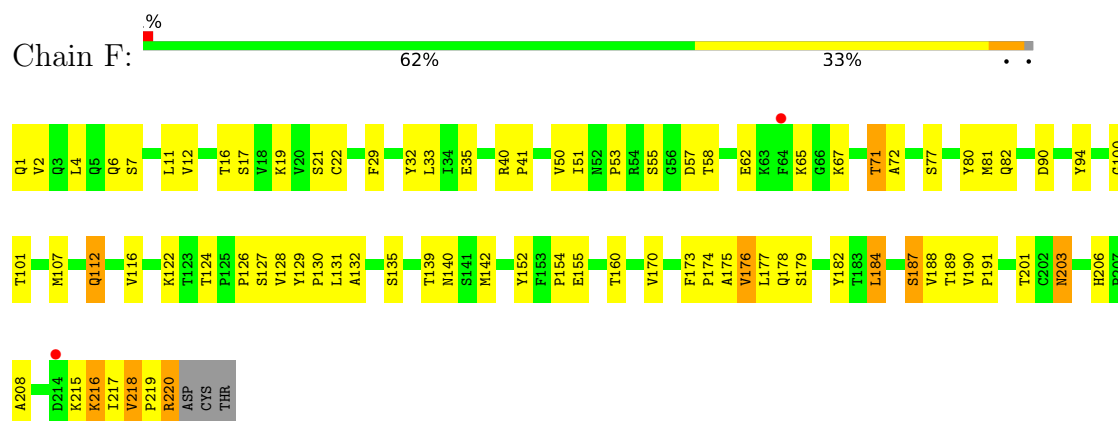
- Molecule 3 is a protein called Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	315	Total	C	N	O	S	0	0	0
			2434	1550	413	462	9			
3	B	309	Total	C	N	O	S	0	0	0
			2397	1528	407	453	9			

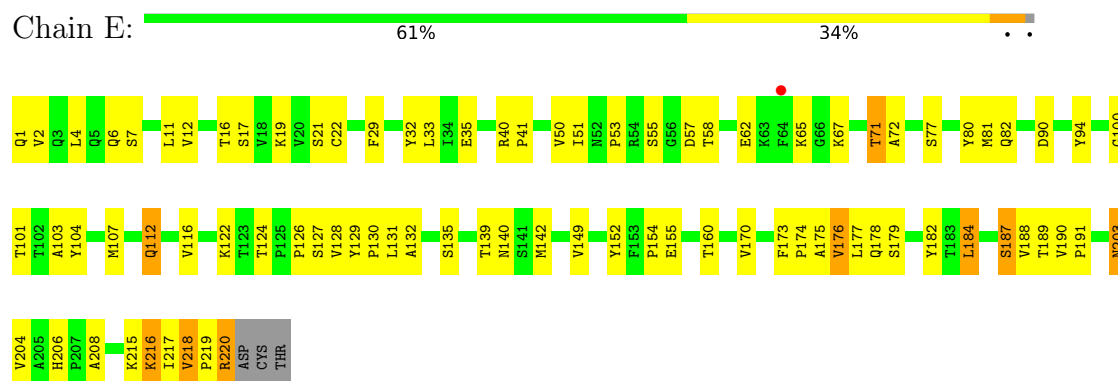
3 Residue-property plots [i](#)

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.

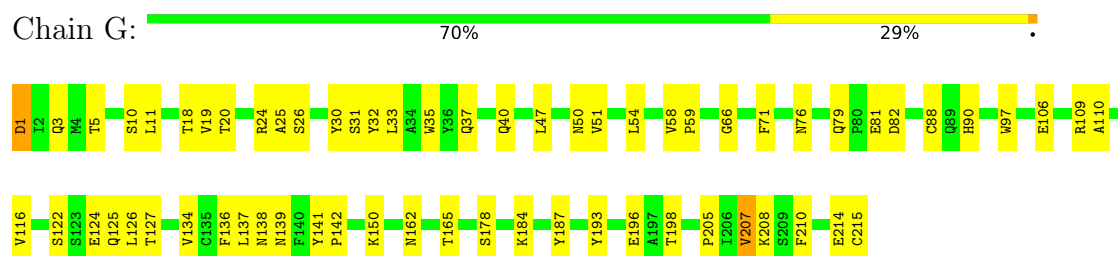
• Molecule 1: 5B18 heavy chain



• Molecule 1: 5B18 heavy chain

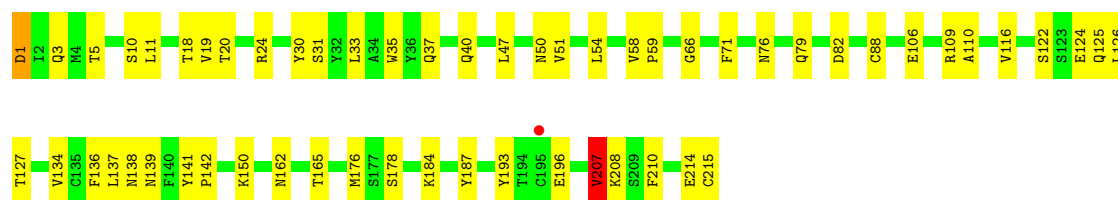


• Molecule 2: 5B18 kappa chain



• Molecule 2: 5B18 kappa chain

Chain H:  73% 26%



• Molecule 3: Capsid

Chain A:  70% 29%



• Molecule 3: Capsid

Chain B:  71% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.48Å 145.48Å 216.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.54 – 3.30 31.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (31.54-3.30) 86.5 (31.54-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_755)	Depositor
R, R_{free}	0.227 , 0.283 0.218 , 0.275	Depositor DCC
R_{free} test set	1540 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11459	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9713e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	E	0.33	0/1683	0.72	0/2300
1	F	0.33	0/1683	0.72	0/2300
2	G	0.32	0/1712	0.75	0/2325
2	H	0.31	0/1712	0.74	1/2325 (0.0%)
3	A	0.35	0/2505	0.80	2/3433 (0.1%)
3	B	0.33	0/2466	0.80	2/3378 (0.1%)
All	All	0.33	0/11761	0.76	5/16061 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	454	ASN	CA-C-N	5.31	125.22	119.76
3	A	454	ASN	C-N-CA	5.31	125.22	119.76
3	B	454	ASN	CA-C-N	5.03	124.94	119.76
3	B	454	ASN	C-N-CA	5.03	124.94	119.76
2	H	207	VAL	N-CA-C	5.01	115.92	108.46

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	E	1643	0	1615	60	0
1	F	1643	0	1615	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1671	0	1592	44	0
2	H	1671	0	1592	40	1
3	A	2434	0	2356	71	1
3	B	2397	0	2322	69	0
All	All	11459	0	11092	313	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 14.

All (313) 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:11:LEU:HD21	2:H:19:VAL:HG21	1.53	0.89
2:G:11:LEU:HD21	2:G:19:VAL:HG21	1.55	0.88
3:A:446:ILE:O	3:B:341:ARG:NH2	2.10	0.84
3:A:399:LEU:HG	3:A:446:ILE:HG21	1.61	0.83
1:F:1:GLN:HG3	1:F:2:VAL:H	1.43	0.82
3:A:341:ARG:NH1	3:B:454:ASN:OD1	2.13	0.81
3:B:399:LEU:HG	3:B:446:ILE:HG21	1.61	0.81
1:E:1:GLN:HG3	1:E:2:VAL:H	1.46	0.79
1:E:132:ALA:O	1:E:220:ARG:NH1	2.18	0.77
1:F:132:ALA:O	1:F:220:ARG:NH1	2.18	0.76
1:F:71:THR:HG23	1:F:80:TYR:HB2	1.66	0.75
1:E:71:THR:HG23	1:E:80:TYR:HB2	1.67	0.75
3:A:341:ARG:NH2	3:B:446:ILE:O	2.17	0.74
1:F:177:LEU:HD12	1:F:182:TYR:CE1	2.23	0.73
2:G:18:THR:HG23	2:G:76:ASN:HA	1.70	0.73
2:H:18:THR:HG23	2:H:76:ASN:HA	1.71	0.72
1:E:177:LEU:HD12	1:E:182:TYR:CE1	2.24	0.72
1:F:177:LEU:HD12	1:F:182:TYR:HE1	1.54	0.72
3:A:454:ASN:OD1	3:B:341:ARG:NH1	2.18	0.72
3:B:267:THR:OG1	3:B:269:ASP:OD1	2.08	0.72
3:A:267:THR:OG1	3:A:269:ASP:OD1	2.08	0.71
1:E:177:LEU:HD12	1:E:182:TYR:HE1	1.55	0.71
1:F:126:PRO:HB3	1:F:152:TYR:HB3	1.73	0.70
3:B:498:LYS:HD3	3:B:533:TYR:HB3	1.75	0.69
1:E:170:VAL:HG22	1:E:188:VAL:HG23	1.75	0.68
3:A:498:LYS:HD3	3:A:533:TYR:HB3	1.77	0.67
1:E:126:PRO:HB3	1:E:152:TYR:HB3	1.76	0.66
1:F:67:LYS:NZ	1:F:90:ASP:OD2	2.27	0.66
3:A:401:SER:HA	3:A:448:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:VAL:HG22	1:F:188:VAL:HG23	1.77	0.64
3:B:401:SER:HA	3:B:448:LEU:HD23	1.79	0.64
1:F:6:GLN:N	1:F:112:GLN:OE1	2.29	0.64
1:F:176:VAL:HG12	1:F:177:LEU:H	1.63	0.64
3:B:278:LEU:HD12	3:B:278:LEU:H	1.64	0.63
3:B:498:LYS:HG3	3:B:535:LEU:HD11	1.81	0.63
3:A:246:ILE:HD12	3:A:442:PHE:HB3	1.80	0.62
1:E:176:VAL:HG12	1:E:177:LEU:H	1.64	0.62
3:A:498:LYS:HG3	3:A:535:LEU:HD11	1.82	0.62
1:E:6:GLN:N	1:E:112:GLN:OE1	2.31	0.62
3:B:246:ILE:HD12	3:B:442:PHE:HB3	1.82	0.62
1:F:55:SER:OG	1:F:57:ASP:OD2	2.12	0.61
3:A:278:LEU:HD12	3:A:278:LEU:H	1.66	0.61
1:F:32:TYR:CD1	1:F:100:GLY:HA3	2.36	0.60
1:F:19:LYS:HG3	1:F:82:GLN:HG2	1.84	0.60
3:A:275:THR:HG23	3:A:322:PRO:HG2	1.83	0.60
1:E:32:TYR:CD1	1:E:100:GLY:HA3	2.36	0.60
3:B:275:THR:HG23	3:B:322:PRO:HG2	1.83	0.60
1:F:173:PHE:CD1	2:G:165:THR:HG23	2.37	0.59
2:G:37:GLN:HB2	2:G:47:LEU:HD11	1.83	0.59
1:E:19:LYS:HG3	1:E:82:GLN:HG2	1.84	0.59
1:F:16:THR:HG22	1:F:17:SER:H	1.68	0.59
1:E:16:THR:HG22	1:E:17:SER:H	1.68	0.59
1:E:35:GLU:HG2	1:E:50:VAL:HG23	1.83	0.59
1:F:35:GLU:HG2	1:F:50:VAL:HG23	1.84	0.58
1:F:7:SER:HB3	1:F:21:SER:OG	2.03	0.58
1:E:155:GLU:HG3	1:E:182:TYR:CD2	2.39	0.58
1:E:129:TYR:HB3	2:H:122:SER:OG	2.04	0.57
3:B:321:VAL:HG13	3:B:322:PRO:HD2	1.87	0.57
3:B:437:GLU:OE2	3:B:498:LYS:HE2	2.05	0.57
1:F:62:GLU:HA	1:F:65:LYS:HB2	1.86	0.57
1:E:62:GLU:HA	1:E:65:LYS:HB2	1.87	0.56
3:A:342:ASN:ND2	3:A:354:ALA:HB3	2.20	0.56
3:B:275:THR:CG2	3:B:322:PRO:HG2	2.35	0.56
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.86	0.56
1:F:155:GLU:HG3	1:F:182:TYR:CD2	2.41	0.56
1:E:16:THR:HG22	1:E:17:SER:N	2.21	0.56
3:A:478:SER:OG	3:A:529:VAL:O	2.19	0.56
1:F:206:HIS:NE2	1:F:208:ALA:HB3	2.20	0.56
1:F:16:THR:HG22	1:F:17:SER:N	2.21	0.55
3:A:324:PRO:O	3:A:327:THR:OG1	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:ARG:HG2	2:G:110:ALA:N	2.20	0.55
2:H:109:ARG:HG2	2:H:110:ALA:N	2.20	0.55
3:A:321:VAL:HG13	3:A:322:PRO:HD2	1.88	0.55
3:B:383:THR:O	3:B:384:GLN:HG3	2.06	0.55
1:E:173:PHE:CD1	2:H:165:THR:HG23	2.41	0.55
3:A:437:GLU:OE2	3:A:498:LYS:HE2	2.06	0.55
3:A:383:THR:O	3:A:384:GLN:HG3	2.07	0.55
3:B:448:LEU:HD11	3:B:455:PRO:CD	2.37	0.55
1:E:35:GLU:OE1	1:E:107:MET:HE2	2.06	0.55
3:A:266:CYS:HB3	3:A:461:MET:HE3	1.89	0.55
1:E:174:PRO:HD3	2:H:165:THR:HG22	1.89	0.55
1:F:35:GLU:OE1	1:F:107:MET:HE2	2.07	0.54
3:A:275:THR:CG2	3:A:322:PRO:HG2	2.36	0.54
3:A:322:PRO:HD3	3:A:425:ASN:O	2.08	0.54
1:F:1:GLN:CG	1:F:2:VAL:H	2.18	0.54
1:E:7:SER:HB3	1:E:21:SER:OG	2.07	0.54
3:B:478:SER:OG	3:B:529:VAL:O	2.21	0.54
3:B:321:VAL:CG1	3:B:322:PRO:HD2	2.38	0.54
2:G:35:TRP:CZ3	2:G:88:CYS:HB3	2.43	0.54
3:B:266:CYS:HB3	3:B:461:MET:HE3	1.91	0.53
1:E:206:HIS:NE2	1:E:208:ALA:HB3	2.24	0.53
3:A:448:LEU:HD11	3:A:455:PRO:CD	2.39	0.53
3:B:244:LEU:HD11	3:B:446:ILE:HG12	1.90	0.53
1:F:122:LYS:O	1:F:124:THR:HG23	2.09	0.53
1:E:178:GLN:O	1:E:179:SER:OG	2.24	0.53
2:H:35:TRP:CZ3	2:H:88:CYS:HB3	2.43	0.53
1:F:187:SER:HB2	2:G:136:PHE:CE2	2.44	0.53
3:A:484:ARG:HB3	3:A:493:THR:HG23	1.91	0.53
1:E:55:SER:OG	1:E:57:ASP:OD2	2.12	0.53
3:B:342:ASN:ND2	3:B:354:ALA:HB3	2.24	0.53
3:B:322:PRO:HD3	3:B:425:ASN:O	2.09	0.52
2:G:214:GLU:O	2:G:215:CYS:HB2	2.09	0.52
3:B:253:PRO:HD2	3:B:512:ALA:HB2	1.92	0.52
2:G:109:ARG:NH1	2:G:110:ALA:O	2.42	0.52
3:B:336:GLY:HA2	3:B:397:VAL:HG23	1.92	0.52
2:H:214:GLU:O	2:H:215:CYS:HB2	2.10	0.52
1:E:71:THR:OG1	1:E:72:ALA:N	2.43	0.51
3:A:336:GLY:HA2	3:A:397:VAL:HG23	1.91	0.51
3:A:253:PRO:HD2	3:A:512:ALA:HB2	1.92	0.51
1:F:51:ILE:O	1:F:53:PRO:HD3	2.10	0.51
3:A:248:VAL:HG11	3:A:514:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:478:SER:HB3	3:B:528:TRP:CE3	2.45	0.51
3:B:484:ARG:HB3	3:B:493:THR:HG23	1.92	0.51
1:E:122:LYS:O	1:E:124:THR:HG23	2.11	0.51
3:A:321:VAL:CG1	3:A:322:PRO:HD2	2.40	0.51
1:E:1:GLN:CG	1:E:2:VAL:H	2.20	0.51
3:A:234:LEU:HD11	3:A:249:LEU:HG	1.92	0.51
3:A:238:THR:HG22	3:B:279:LEU:HD22	1.92	0.51
1:F:71:THR:OG1	1:F:72:ALA:N	2.43	0.50
3:A:266:CYS:HB3	3:A:461:MET:CE	2.41	0.50
2:G:11:LEU:HD21	2:G:19:VAL:CG2	2.35	0.50
3:B:399:LEU:O	3:B:448:LEU:HA	2.12	0.50
1:E:129:TYR:CE1	2:H:125:GLN:HA	2.47	0.50
2:H:50:ASN:O	2:H:51:VAL:HB	2.11	0.50
3:B:242:PHE:O	3:B:244:LEU:N	2.44	0.50
3:B:478:SER:OG	3:B:479:ASP:N	2.45	0.50
2:H:196:GLU:HG2	2:H:207:VAL:CG1	2.41	0.50
3:B:234:LEU:HD11	3:B:249:LEU:HG	1.93	0.50
1:E:128:VAL:O	1:E:215:LYS:HE2	2.12	0.50
3:B:266:CYS:HB3	3:B:461:MET:CE	2.42	0.50
3:B:340:GLN:NE2	3:B:390:GLN:HB2	2.26	0.50
2:G:116:VAL:O	2:G:208:LYS:HG3	2.12	0.50
3:A:340:GLN:NE2	3:A:390:GLN:HB2	2.27	0.50
2:G:196:GLU:HG2	2:G:207:VAL:CG1	2.42	0.50
3:A:399:LEU:O	3:A:448:LEU:HA	2.12	0.49
3:A:481:ALA:HB3	3:A:499:LEU:HB3	1.94	0.49
3:A:478:SER:HB3	3:A:528:TRP:CE3	2.47	0.49
2:G:32:TYR:OH	3:B:535:LEU:O	2.17	0.49
3:B:480:VAL:HG12	3:B:529:VAL:HG23	1.94	0.49
2:G:109:ARG:HG2	2:G:110:ALA:H	1.77	0.49
2:H:109:ARG:NH1	2:H:110:ALA:O	2.45	0.49
3:A:244:LEU:HD11	3:A:446:ILE:HG12	1.93	0.49
3:A:480:VAL:HG12	3:A:529:VAL:HG23	1.93	0.49
3:B:442:PHE:HB2	3:B:459:CYS:SG	2.53	0.49
2:G:50:ASN:O	2:G:51:VAL:HB	2.12	0.49
2:H:11:LEU:HD21	2:H:19:VAL:CG2	2.34	0.49
2:H:1:ASP:O	2:H:3:GLN:HG3	2.13	0.49
3:A:442:PHE:HB2	3:A:459:CYS:SG	2.53	0.49
3:B:248:VAL:HG11	3:B:514:PRO:HB3	1.95	0.49
1:E:51:ILE:O	1:E:53:PRO:HD3	2.12	0.49
2:H:109:ARG:HG2	2:H:110:ALA:H	1.78	0.49
3:A:224:SER:O	3:A:224:SER:OG	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:484:ARG:HB3	3:A:493:THR:CG2	2.43	0.49
2:H:162:ASN:OD1	2:H:178:SER:HB2	2.13	0.48
3:A:448:LEU:HD12	3:B:341:ARG:NH2	2.27	0.48
3:A:437:GLU:OE1	3:A:506:THR:HG21	2.13	0.48
1:F:131:LEU:HD11	2:G:134:VAL:HG21	1.95	0.48
1:F:218:VAL:HG23	1:F:219:PRO:O	2.13	0.48
1:E:142:MET:HE3	1:E:189:THR:HG22	1.96	0.48
2:G:162:ASN:OD1	2:G:178:SER:HB2	2.13	0.48
1:E:51:ILE:HG13	1:E:58:THR:HG22	1.96	0.48
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.49	0.48
3:B:268:LEU:HA	3:B:469:LEU:HD13	1.95	0.48
1:F:51:ILE:HG13	1:F:58:THR:HG22	1.96	0.48
1:F:129:TYR:CE1	2:G:125:GLN:HA	2.49	0.48
2:H:5:THR:HB	2:H:24:ARG:HB3	1.96	0.48
3:A:268:LEU:HA	3:A:469:LEU:HD13	1.95	0.48
1:E:4:LEU:HD22	1:E:22:CYS:SG	2.54	0.48
3:A:242:PHE:O	3:A:244:LEU:N	2.47	0.47
3:B:484:ARG:HB3	3:B:493:THR:CG2	2.44	0.47
1:E:160:THR:OG1	1:E:203:ASN:OD1	2.32	0.47
2:G:1:ASP:O	2:G:3:GLN:HG3	2.14	0.47
1:E:33:LEU:HD13	3:A:435:PRO:HG2	1.97	0.47
1:F:4:LEU:HD22	1:F:22:CYS:SG	2.55	0.47
1:E:218:VAL:HG23	1:E:219:PRO:O	2.14	0.47
2:H:126:LEU:O	2:H:184:LYS:HD3	2.14	0.47
3:A:238:THR:HG21	3:B:280:PRO:HD2	1.97	0.47
1:F:184:LEU:HD23	1:F:184:LEU:C	2.40	0.47
1:E:67:LYS:NZ	1:E:90:ASP:OD2	2.29	0.47
1:F:128:VAL:O	1:F:215:LYS:HE2	2.15	0.47
1:F:40:ARG:HB3	1:F:41:PRO:HD2	1.97	0.47
2:G:66:GLY:HA3	2:G:71:PHE:HA	1.96	0.47
2:G:187:TYR:O	2:G:193:TYR:OH	2.32	0.47
1:E:130:PRO:HG3	1:E:215:LYS:HB3	1.97	0.47
2:H:116:VAL:O	2:H:208:LYS:HG3	2.15	0.47
1:F:130:PRO:HG3	1:F:215:LYS:HB3	1.96	0.46
1:F:142:MET:HE3	1:F:189:THR:HG22	1.97	0.46
1:F:81:MET:HE1	1:F:94:TYR:CD1	2.51	0.46
1:F:160:THR:OG1	1:F:203:ASN:OD1	2.33	0.46
1:F:129:TYR:HB3	2:G:122:SER:OG	2.15	0.46
2:G:126:LEU:O	2:G:184:LYS:HD3	2.15	0.46
2:H:66:GLY:HA3	2:H:71:PHE:HA	1.96	0.46
3:A:453:GLY:HA2	3:B:352:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:LEU:HD11	1:F:154:PRO:HG3	1.98	0.46
1:E:81:MET:HE1	1:E:94:TYR:CD1	2.51	0.46
3:B:437:GLU:OE1	3:B:506:THR:HG21	2.15	0.46
2:G:122:SER:HB2	2:G:124:GLU:OE2	2.16	0.46
3:A:266:CYS:O	3:A:503:GLY:HA3	2.16	0.46
2:G:58:VAL:HA	2:G:59:PRO:HD3	1.84	0.46
1:F:130:PRO:HB3	1:F:217:ILE:HD13	1.96	0.46
2:G:214:GLU:O	2:G:215:CYS:CB	2.64	0.46
2:H:187:TYR:O	2:H:193:TYR:OH	2.31	0.46
1:E:40:ARG:HB3	1:E:41:PRO:HD2	1.98	0.45
2:H:214:GLU:O	2:H:215:CYS:CB	2.64	0.45
3:B:230:PRO:HG3	3:B:468:HIS:CB	2.46	0.45
2:G:33:LEU:HD22	2:G:71:PHE:CG	2.51	0.45
2:G:5:THR:HB	2:G:24:ARG:HB3	1.98	0.45
1:E:139:THR:CG2	1:E:140:ASN:N	2.78	0.45
3:A:249:LEU:O	3:A:515:VAL:N	2.48	0.45
1:F:33:LEU:HD13	3:B:435:PRO:HG2	1.98	0.45
2:G:150:LYS:HD2	2:G:196:GLU:CD	2.42	0.45
2:H:122:SER:HB2	2:H:124:GLU:OE2	2.15	0.45
3:A:478:SER:OG	3:A:479:ASP:N	2.49	0.45
2:G:54:LEU:HD21	2:G:58:VAL:O	2.17	0.45
1:E:130:PRO:HB3	1:E:217:ILE:HD13	1.98	0.45
3:A:294:VAL:N	3:A:302:HIS:O	2.45	0.45
3:B:266:CYS:O	3:B:503:GLY:HA3	2.17	0.45
3:B:481:ALA:HB3	3:B:499:LEU:HB3	1.97	0.45
2:H:30:TYR:O	2:H:31:SER:HB2	2.16	0.45
3:B:249:LEU:O	3:B:515:VAL:N	2.48	0.45
3:A:277:GLN:HG2	3:A:278:LEU:N	2.32	0.45
2:G:18:THR:HG22	2:G:19:VAL:N	2.32	0.44
1:F:190:VAL:HB	1:F:191:PRO:HD2	1.98	0.44
2:H:141:TYR:CG	2:H:142:PRO:HA	2.52	0.44
3:A:448:LEU:HD12	3:B:341:ARG:HH21	1.82	0.44
1:F:32:TYR:CE1	1:F:100:GLY:HA3	2.53	0.44
1:F:71:THR:CG2	1:F:80:TYR:HB2	2.42	0.44
1:E:50:VAL:HG22	1:E:51:ILE:N	2.33	0.44
1:E:187:SER:HB2	2:H:136:PHE:CE2	2.53	0.44
3:A:234:LEU:HD22	3:A:519:THR:HG22	2.00	0.44
2:G:141:TYR:CG	2:G:142:PRO:HA	2.52	0.44
1:E:35:GLU:HG2	1:E:50:VAL:CG2	2.48	0.44
1:F:139:THR:CG2	1:F:140:ASN:N	2.80	0.44
1:E:32:TYR:CE1	1:E:100:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:LYS:HD2	2:H:196:GLU:CD	2.42	0.44
2:H:162:ASN:HB3	2:H:176:MET:HE3	2.00	0.44
2:G:136:PHE:O	2:G:137:LEU:HD12	2.18	0.43
3:A:434:PHE:HA	3:A:435:PRO:HD3	1.90	0.43
1:E:190:VAL:HB	1:E:191:PRO:HD2	1.99	0.43
3:A:401:SER:HB2	3:A:403:ASP:OD1	2.18	0.43
2:H:19:VAL:HG22	2:H:20:THR:N	2.31	0.43
2:H:54:LEU:HD21	2:H:58:VAL:O	2.18	0.43
2:H:58:VAL:HA	2:H:59:PRO:HD3	1.84	0.43
2:H:18:THR:HG22	2:H:19:VAL:N	2.32	0.43
1:F:29:PHE:CD2	1:F:77:SER:HA	2.53	0.43
3:A:449:LYS:HA	3:B:357:ALA:HB3	2.00	0.43
1:F:178:GLN:O	1:F:179:SER:OG	2.28	0.43
3:A:279:LEU:HD22	3:B:238:THR:HG22	2.01	0.43
2:G:30:TYR:O	2:G:31:SER:HB2	2.19	0.43
3:A:342:ASN:HA	3:A:390:GLN:OE1	2.19	0.43
3:B:323:ALA:HB1	3:B:324:PRO:HD2	2.01	0.43
2:G:81:GLU:OE1	2:G:81:GLU:N	2.38	0.43
2:H:210:PHE:CD1	2:H:210:PHE:C	2.97	0.43
3:A:230:PRO:HG3	3:A:468:HIS:CB	2.48	0.43
3:B:230:PRO:HG3	3:B:468:HIS:CG	2.54	0.43
3:B:324:PRO:O	3:B:327:THR:OG1	2.14	0.42
3:B:401:SER:HB2	3:B:403:ASP:OD1	2.19	0.42
3:A:266:CYS:O	3:A:461:MET:HE1	2.19	0.42
3:B:324:PRO:HD2	3:B:371:PRO:HB2	2.01	0.42
1:F:57:ASP:OD2	3:B:531:GLN:HG2	2.18	0.42
1:E:152:TYR:OH	1:E:175:ALA:HB2	2.20	0.42
3:B:322:PRO:HB3	3:B:426:LEU:HD23	2.00	0.42
3:A:324:PRO:HD2	3:A:371:PRO:HB2	2.02	0.42
2:G:79:GLN:O	2:G:82:ASP:HB2	2.20	0.42
1:E:11:LEU:HD11	1:E:154:PRO:HG3	2.00	0.42
3:A:323:ALA:HB1	3:A:324:PRO:HD2	2.01	0.42
3:B:277:GLN:HG2	3:B:278:LEU:N	2.33	0.42
2:G:19:VAL:HG22	2:G:20:THR:N	2.34	0.42
3:A:308:THR:HB	3:A:313:THR:O	2.19	0.42
3:A:322:PRO:HB3	3:A:426:LEU:HD23	2.01	0.42
2:G:25:ALA:O	2:G:26:SER:C	2.63	0.42
3:B:234:LEU:HD22	3:B:519:THR:HG22	2.02	0.42
2:G:138:ASN:HB3	2:G:139:ASN:OD1	2.20	0.42
3:B:238:THR:HB	3:B:244:LEU:O	2.20	0.41
3:B:322:PRO:O	3:B:372:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:TYR:HA	1:F:130:PRO:HD3	1.86	0.41
1:F:152:TYR:OH	1:F:175:ALA:HB2	2.20	0.41
1:E:29:PHE:CD2	1:E:77:SER:HA	2.55	0.41
1:E:184:LEU:C	1:E:184:LEU:HD23	2.45	0.41
2:H:138:ASN:HB3	2:H:139:ASN:OD1	2.20	0.41
1:E:1:GLN:OE1	1:E:1:GLN:HA	2.21	0.41
1:E:149:VAL:HG22	1:E:204:VAL:HG21	2.03	0.41
2:H:79:GLN:O	2:H:82:ASP:HB2	2.21	0.41
1:F:174:PRO:HD3	2:G:165:THR:HG22	2.02	0.41
2:G:210:PHE:CD1	2:G:210:PHE:C	2.99	0.41
1:E:216:LYS:NZ	1:E:216:LYS:HB2	2.35	0.41
2:H:136:PHE:O	2:H:137:LEU:HD12	2.20	0.41
2:G:198:THR:HG22	2:G:205:PRO:HB3	2.02	0.41
3:A:409:ASP:OD2	3:A:412:THR:HG23	2.21	0.41
3:A:505:LEU:HD23	3:A:505:LEU:HA	1.86	0.41
1:E:71:THR:CG2	1:E:80:TYR:HB2	2.43	0.41
1:E:135:SER:HB2	2:H:214:GLU:HB3	2.03	0.41
1:F:50:VAL:HG22	1:F:51:ILE:N	2.36	0.41
1:F:130:PRO:HG3	1:F:215:LYS:HE3	2.02	0.41
3:B:352:LEU:HA	3:B:353:PRO:HD3	1.90	0.41
3:B:505:LEU:HA	3:B:505:LEU:HD23	1.86	0.41
1:E:131:LEU:HD11	2:H:134:VAL:HG21	2.03	0.41
3:B:266:CYS:O	3:B:461:MET:HE1	2.21	0.41
1:E:103:ALA:O	1:E:104:TYR:C	2.64	0.40
1:E:139:THR:HG22	1:E:140:ASN:N	2.36	0.40
3:A:238:THR:HB	3:A:244:LEU:O	2.21	0.40
3:A:472:GLU:O	3:A:473:SER:C	2.64	0.40
1:F:135:SER:HB2	2:G:214:GLU:HB3	2.03	0.40
1:F:201:THR:HG23	1:F:216:LYS:HA	2.03	0.40
3:B:278:LEU:HD12	3:B:278:LEU:N	2.34	0.40
3:A:392:THR:HG22	3:A:393:LYS:N	2.37	0.40
1:F:130:PRO:CG	1:F:215:LYS:HE3	2.51	0.40
1:E:6:GLN:HA	1:E:21:SER:O	2.21	0.40
3:A:338:ILE:HG23	3:A:392:THR:HG23	2.04	0.40
2:G:90:HIS:O	2:G:97:TRP:HB3	2.21	0.40
3:A:474:ALA:HA	3:A:475:PRO:HD3	1.93	0.40
3:B:308:THR:HB	3:B:313:THR:O	2.21	0.40
3:B:472:GLU:O	3:B:473:SER:C	2.65	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)
2:H:150:LYS:NZ	3:A:271:GLU:OE1[3_644]	2.11	0.09

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	218/223 (98%)	194 (89%)	24 (11%)	0	100	100
1	F	218/223 (98%)	194 (89%)	24 (11%)	0	100	100
2	G	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
2	H	213/215 (99%)	194 (91%)	19 (9%)	0	100	100
3	A	313/315 (99%)	295 (94%)	17 (5%)	1 (0%)	36	65
3	B	305/315 (97%)	288 (94%)	16 (5%)	1 (0%)	36	65
All	All	1480/1506 (98%)	1358 (92%)	120 (8%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	243	PRO
3	B	243	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	187/190 (98%)	174 (93%)	13 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	187/190 (98%)	174 (93%)	13 (7%)	14	41
2	G	190/190 (100%)	184 (97%)	6 (3%)	34	60
2	H	190/190 (100%)	184 (97%)	6 (3%)	34	60
3	A	270/270 (100%)	257 (95%)	13 (5%)	23	52
3	B	266/270 (98%)	254 (96%)	12 (4%)	24	53
All	All	1290/1300 (99%)	1227 (95%)	63 (5%)	22	51

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	12	VAL
1	F	71	THR
1	F	101	THR
1	F	112	GLN
1	F	116	VAL
1	F	127	SER
1	F	176	VAL
1	F	184	LEU
1	F	187	SER
1	F	203	ASN
1	F	216	LYS
1	F	218	VAL
1	F	220	ARG
2	G	1	ASP
2	G	10	SER
2	G	40	GLN
2	G	106	GLU
2	G	127	THR
2	G	207	VAL
1	E	12	VAL
1	E	71	THR
1	E	101	THR
1	E	112	GLN
1	E	116	VAL
1	E	127	SER
1	E	176	VAL
1	E	184	LEU
1	E	187	SER
1	E	203	ASN
1	E	216	LYS

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Mol	Chain	Res	Type
1	E	218	VAL
1	E	220	ARG
2	H	1	ASP
2	H	10	SER
2	H	40	GLN
2	H	106	GLU
2	H	127	THR
2	H	207	VAL
3	A	248	VAL
3	A	261	CYS
3	A	277	GLN
3	A	278	LEU
3	A	318	THR
3	A	359	GLU
3	A	417	SER
3	A	433	VAL
3	A	471	GLN
3	A	479	ASP
3	A	490	THR
3	A	516	VAL
3	A	538	MET
3	B	248	VAL
3	B	261	CYS
3	B	277	GLN
3	B	278	LEU
3	B	318	THR
3	B	417	SER
3	B	433	VAL
3	B	471	GLN
3	B	479	ASP
3	B	490	THR
3	B	516	VAL
3	B	538	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	471	GLN
3	B	273	GLN

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 [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	E	220/223 (98%)	-0.17	1 (0%) 87 76	56, 82, 111, 156	0
1	F	220/223 (98%)	-0.25	2 (0%) 81 65	54, 82, 110, 157	0
2	G	215/215 (100%)	-0.20	0 100 100	61, 84, 116, 143	0
2	H	215/215 (100%)	-0.20	1 (0%) 87 76	60, 85, 116, 144	0
3	A	315/315 (100%)	-0.11	1 (0%) 90 82	52, 77, 120, 179	0
3	B	309/315 (98%)	-0.23	0 100 100	54, 78, 116, 180	0
All	All	1494/1506 (99%)	-0.19	5 (0%) 90 82	52, 81, 116, 180	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	360	ALA	2.6
1	F	64	PHE	2.5
1	E	64	PHE	2.4
1	F	214	ASP	2.4
2	H	195	CYS	2.3

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.