Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 12:04 pm BST

PDB ID	:	1W7P
Title	:	The crystal structure of endosomal complex ESCRT-II (VPS22/VPS25/VPS36)
Authors	:	Teo, H.; Perisic, O.; Gonzalez, B.; Williams, R.L.
Deposited on	:	2004-09-07
Resolution	:	3.60 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 (i) 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 (1)) were used in the production of this report:

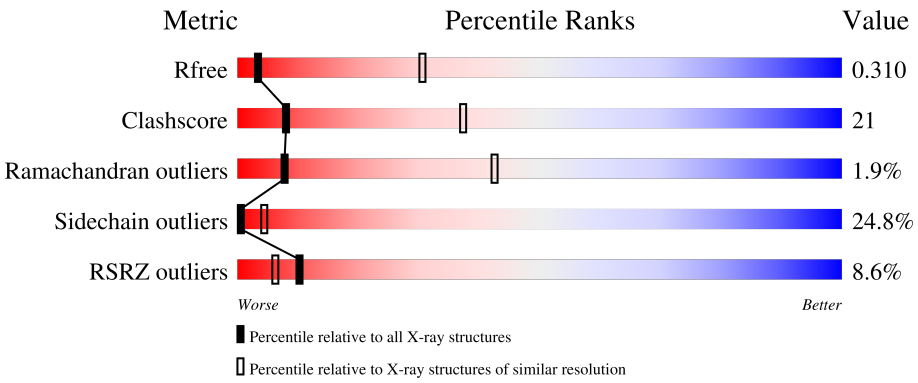
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	%, 52%, 33%, 7%, 9%
2	B	202	12%, 38%, 40%, 12%, 10%
2	C	202	16%, 38%, 39%, 11%, •, 10%
3	D	566	%, 15%, 12%, •, 70%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6134 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 VPS22, YPL002C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	1732	1108	290	323	11	0	0	0

- Molecule 2 is a protein called VPS25, YJR102C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	182	1504	959	252	284	9	0	0	0
2	C	182	1504	959	252	284	9	0	0	0

- Molecule 3 is a protein called VPS36P, YLR417W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	171	1394	891	226	268	9	0	0	0

3 Residue-property plots (i)

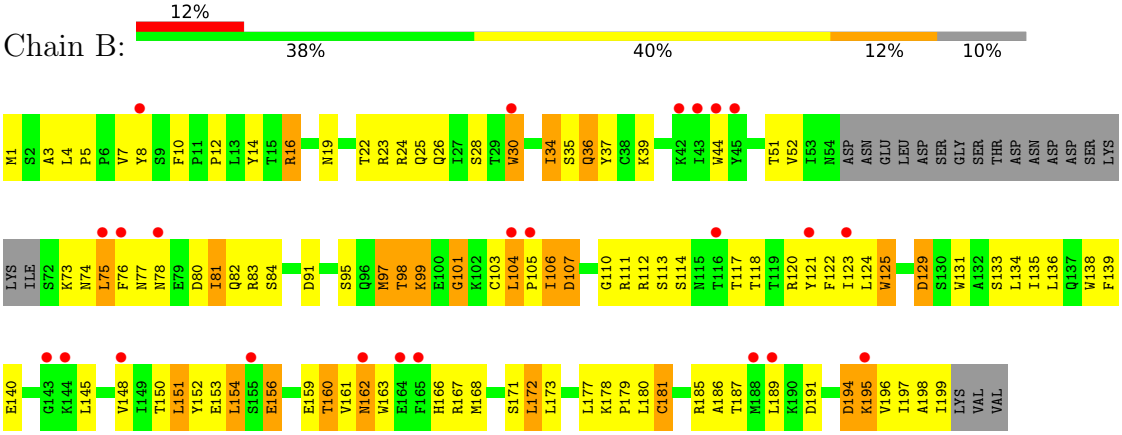
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VPS22, YPL002C

Chain A:

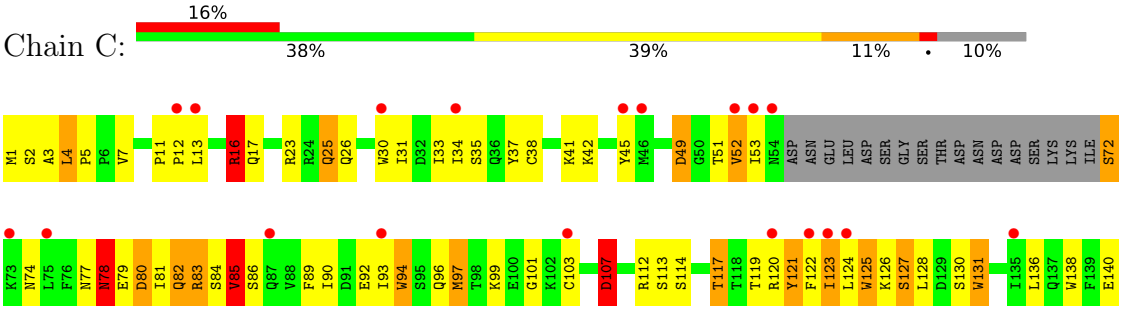
- Molecule 2: VPS25, YJR102C

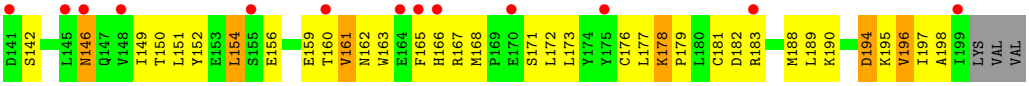
Chain B:



- Molecule 2: VPS25, YJR102C

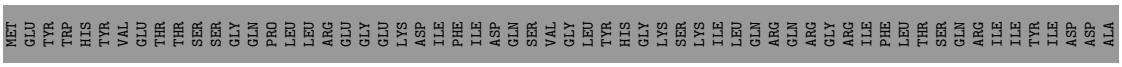
Chain C:

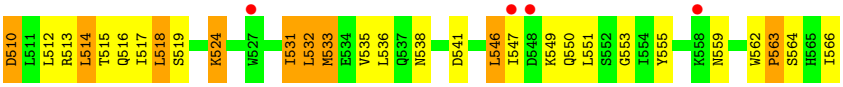




• Molecule 3: VPS36P, YLR417W

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	149.91Å 149.91Å 186.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.06 – 3.60 92.11 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (92.06-3.60) 99.0 (92.11-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.292 , 0.330 0.272 , 0.310	Depositor DCC
R_{free} test set	1216 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	141.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 159.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6134	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.80	0/1764	0.88	6/2372 (0.3%)
2	B	0.68	0/1539	0.91	5/2087 (0.2%)
2	C	0.75	0/1539	0.94	5/2087 (0.2%)
3	D	0.85	0/1416	0.95	4/1908 (0.2%)
All	All	0.77	0/6258	0.92	20/8454 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	425	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	168	ASP	CB-CG-OD2	6.91	124.52	118.30
2	C	107	ASP	CB-CG-OD2	6.73	124.36	118.30
3	D	501	ASP	CB-CG-OD2	6.44	124.09	118.30
3	D	510	ASP	CB-CG-OD2	6.43	124.09	118.30
2	C	49	ASP	CB-CG-OD2	6.23	123.91	118.30
2	B	194	ASP	CB-CG-OD2	5.89	123.60	118.30
3	D	541	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	132	ASP	CB-CG-OD2	5.76	123.48	118.30
2	C	194	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	90	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	133	ASP	CB-CG-OD2	5.62	123.36	118.30
2	C	80	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	107	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	191	ASP	CB-CG-OD2	5.54	123.29	118.30
2	C	85	VAL	N-CA-C	5.47	125.77	111.00
2	B	129	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	34	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	108	ASP	CB-CG-OD2	5.03	122.82	118.30
2	B	91	ASP	CB-CG-OD2	5.02	122.81	118.30

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	1732	0	1741	51	0
2	B	1504	0	1487	80	0
2	C	1504	0	1487	93	0
3	D	1394	0	1406	47	0
All	All	6134	0	6121	262	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 21.

All (262) 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:C:74:ASN:O	2:C:78:ASN:HB3	1.46	1.16
2:C:94:TRP:CE2	2:C:121:TYR:CD2	2.58	0.92
2:C:122:PHE:CZ	2:C:172:LEU:HD22	2.06	0.90
2:B:186:ALA:HB1	2:B:199:ILE:HA	1.57	0.86
2:C:122:PHE:CE2	2:C:172:LEU:HD22	2.11	0.84
2:C:74:ASN:O	2:C:78:ASN:CB	2.27	0.83
2:C:77:ASN:OD1	2:C:84:SER:HB3	1.81	0.80
2:B:51:THR:HG23	2:B:74:ASN:HD21	1.49	0.78
2:C:77:ASN:OD1	2:C:84:SER:CB	2.32	0.78
1:A:161:VAL:HB	1:A:162:PRO:CD	2.16	0.75
2:C:160:THR:HG23	2:C:166:HIS:CG	2.21	0.75
2:C:94:TRP:CG	2:C:121:TYR:CE2	2.75	0.74
2:C:94:TRP:CD2	2:C:121:TYR:CE2	2.78	0.71
2:B:74:ASN:O	2:B:78:ASN:N	2.23	0.70
3:D:441:TYR:HD2	3:D:460:MET:HG3	1.55	0.70
1:A:202:LEU:HG	1:A:223:TYR:CD1	2.26	0.70
2:C:161:VAL:HG12	2:C:162:ASN:H	1.59	0.68
3:D:435:ILE:HG22	3:D:436:THR:O	1.93	0.68
3:D:434:ILE:HG23	3:D:488:THR:HG22	1.75	0.68
3:D:562:TRP:HB3	3:D:563:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:HD12	2:B:196:VAL:HG23	1.75	0.67
2:C:94:TRP:CD2	2:C:121:TYR:CD2	2.84	0.66
2:B:166:HIS:O	2:B:167:ARG:HB2	1.95	0.65
3:D:455:ILE:HG23	3:D:459:GLU:HG3	1.77	0.65
2:B:74:ASN:O	2:B:78:ASN:HB2	1.97	0.64
2:B:136:LEU:O	2:B:140:GLU:CB	2.47	0.63
2:B:148:VAL:HG13	2:B:198:ALA:HB2	1.81	0.63
2:B:136:LEU:O	2:B:140:GLU:HB2	1.99	0.63
2:C:146:ASN:N	2:C:146:ASN:HD22	1.97	0.63
2:B:173:LEU:O	2:B:177:LEU:HD23	2.00	0.62
2:C:127:SER:O	2:C:131:TRP:HB2	1.99	0.62
2:C:25:GLN:HG2	3:D:563:PRO:HD3	1.82	0.62
1:A:121:LYS:NZ	1:A:232:GLN:HE22	1.98	0.61
2:B:161:VAL:HB	2:B:163:TRP:HD1	1.65	0.61
2:B:51:THR:HG23	2:B:74:ASN:ND2	2.16	0.61
2:C:83:ARG:CG	2:C:83:ARG:HH11	2.14	0.61
2:C:166:HIS:O	2:C:167:ARG:HB2	2.01	0.60
1:A:224:TRP:CD1	2:B:12:PRO:HG3	2.36	0.60
2:B:51:THR:HA	2:B:74:ASN:ND2	2.16	0.60
1:A:186:LEU:HD23	1:A:190:ASN:ND2	2.17	0.59
2:B:135:ILE:HG22	2:B:139:PHE:CE1	2.37	0.59
2:C:77:ASN:O	2:C:79:GLU:N	2.35	0.59
2:C:94:TRP:CD1	2:C:121:TYR:CE2	2.91	0.58
2:C:107:ASP:CB	2:C:117:THR:HA	2.33	0.58
2:C:168:MET:SD	2:C:172:LEU:HD23	2.42	0.58
1:A:227:SER:O	1:A:228:TRP:C	2.42	0.58
2:B:5:PRO:O	2:B:8:TYR:HB3	2.03	0.58
2:C:177:LEU:C	2:C:179:PRO:HD2	2.24	0.58
2:C:77:ASN:HA	2:C:84:SER:HB2	1.86	0.58
3:D:510:ASP:HB3	3:D:555:TYR:CD2	2.39	0.58
1:A:198:SER:O	1:A:202:LEU:HB2	2.03	0.57
2:B:122:PHE:CE1	2:B:172:LEU:HD13	2.39	0.57
2:C:168:MET:HB3	2:C:173:LEU:HD21	1.85	0.57
1:A:51:ASN:O	1:A:54:LEU:HB2	2.04	0.57
1:A:51:ASN:O	1:A:54:LEU:CB	2.53	0.57
2:C:85:VAL:HG22	2:C:86:SER:H	1.70	0.57
2:B:37:TYR:CD2	2:B:75:LEU:HD21	2.40	0.57
2:B:189:LEU:HD12	2:B:196:VAL:CG2	2.34	0.56
2:B:34:ILE:HG22	2:B:35:SER:N	2.18	0.56
2:B:103:CYS:HA	2:B:122:PHE:O	2.04	0.56
2:C:79:GLU:OE1	2:C:79:GLU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:ARG:NH2	3:D:550:GLN:HB2	2.20	0.56
3:D:463:ALA:O	3:D:466:ARG:HG2	2.06	0.55
2:C:16:ARG:HH11	2:C:16:ARG:CG	2.19	0.55
2:C:31:ILE:HG12	2:C:97:MET:HG3	1.88	0.55
1:A:185:SER:HB3	1:A:220:GLU:OE1	2.05	0.55
2:B:51:THR:HA	2:B:74:ASN:HD22	1.70	0.55
2:C:77:ASN:HA	2:C:84:SER:CB	2.37	0.55
2:C:13:LEU:HG	2:C:30:TRP:CZ2	2.42	0.55
1:A:146:CYS:SG	3:D:438:VAL:HG21	2.47	0.54
2:C:97:MET:HA	2:C:101:GLY:HA3	1.89	0.54
2:C:107:ASP:HB3	2:C:117:THR:HA	1.88	0.54
3:D:562:TRP:HB3	3:D:563:PRO:CD	2.37	0.54
2:B:154:LEU:HA	2:B:159:GLU:HG3	1.89	0.54
2:C:77:ASN:OD1	2:C:84:SER:OG	2.26	0.53
2:C:83:ARG:CG	2:C:83:ARG:NH1	2.70	0.53
1:A:191:LEU:HD12	1:A:193:TRP:CD1	2.44	0.53
2:C:126:LYS:HD3	2:C:131:TRP:CZ3	2.43	0.53
2:C:16:ARG:HG2	2:C:89:PHE:CE2	2.44	0.53
3:D:480:VAL:HG23	3:D:484:ILE:HB	1.89	0.53
3:D:481:ASN:ND2	3:D:538:ASN:OD1	2.42	0.53
2:C:188:MET:HB2	2:C:197:ILE:HG12	1.90	0.52
2:C:53:ILE:HG12	2:C:72:SER:HB2	1.90	0.52
2:B:172:LEU:O	2:B:173:LEU:C	2.47	0.52
2:B:181:CYS:HB3	2:B:185:ARG:HD3	1.90	0.52
2:C:150:THR:HB	2:C:196:VAL:HG23	1.90	0.52
2:B:52:VAL:HG13	2:B:73:LYS:O	2.10	0.52
2:C:16:ARG:HH11	2:C:16:ARG:HG2	1.74	0.52
2:B:80:ASP:C	2:B:82:GLN:H	2.11	0.52
2:B:122:PHE:C	2:B:123:ILE:HG13	2.30	0.52
2:C:154:LEU:HA	2:C:159:GLU:CG	2.39	0.52
2:B:122:PHE:CE2	2:B:172:LEU:HD22	2.44	0.52
2:C:178:LYS:N	2:C:179:PRO:HD2	2.25	0.52
2:B:74:ASN:O	2:B:78:ASN:CB	2.57	0.52
2:C:178:LYS:O	2:C:181:CYS:SG	2.66	0.52
2:B:122:PHE:O	2:B:123:ILE:HG13	2.09	0.51
2:B:98:THR:HG22	2:B:99:LYS:N	2.24	0.51
2:B:151:LEU:CD1	2:B:195:LYS:HD3	2.41	0.51
2:B:168:MET:HG2	2:B:173:LEU:HG	1.93	0.51
2:C:190:LYS:HB3	2:C:195:LYS:HZ2	1.74	0.51
2:B:37:TYR:CE2	2:B:75:LEU:HD21	2.46	0.51
3:D:514:LEU:HA	3:D:517:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:THR:HB	2:C:196:VAL:CG2	2.41	0.51
1:A:213:ILE:O	2:B:12:PRO:HB3	2.10	0.51
2:B:125:TRP:CE3	2:B:125:TRP:N	2.79	0.51
3:D:404:LYS:O	3:D:407:PHE:HB3	2.11	0.51
1:A:229:ILE:HD11	2:B:10:PHE:CD2	2.46	0.51
3:D:444:TYR:HE2	3:D:455:ILE:CD1	2.24	0.50
1:A:186:LEU:CD2	1:A:190:ASN:ND2	2.73	0.50
2:C:168:MET:SD	2:C:172:LEU:CD2	2.99	0.50
2:B:97:MET:O	2:B:101:GLY:HA3	2.11	0.50
2:B:154:LEU:HA	2:B:159:GLU:CG	2.42	0.50
2:C:151:LEU:HD13	2:C:173:LEU:HB2	1.93	0.50
3:D:406:LEU:O	3:D:406:LEU:HD22	2.11	0.50
2:B:122:PHE:CD1	2:B:172:LEU:HD11	2.47	0.50
3:D:407:PHE:CZ	3:D:411:ILE:HD11	2.46	0.50
2:C:85:VAL:HG22	2:C:86:SER:N	2.26	0.50
2:B:23:ARG:O	2:B:26:GLN:N	2.45	0.50
3:D:480:VAL:HG11	3:D:492:PHE:CG	2.47	0.50
1:A:121:LYS:HZ3	1:A:232:GLN:HE22	1.57	0.49
3:D:416:TYR:CE1	3:D:472:LEU:HB3	2.47	0.49
2:B:44:TRP:HB3	2:B:122:PHE:HE1	1.76	0.49
1:A:118:GLU:HA	1:A:230:THR:HG21	1.93	0.49
1:A:152:ILE:C	1:A:154:GLY:N	2.62	0.49
1:A:191:LEU:HD22	1:A:191:LEU:O	2.12	0.49
2:C:149:ILE:CD1	2:C:154:LEU:HD23	2.41	0.49
2:C:17:GLN:HG2	2:C:26:GLN:HE22	1.78	0.49
2:C:94:TRP:CE2	2:C:121:TYR:CE2	3.01	0.49
2:C:122:PHE:CD2	2:C:123:ILE:N	2.80	0.49
2:C:149:ILE:HD11	2:C:154:LEU:HD23	1.94	0.49
2:C:94:TRP:CZ2	2:C:121:TYR:CD2	3.00	0.49
3:D:398:ARG:HB2	3:D:399:GLU:HG2	1.93	0.49
3:D:532:LEU:HD22	3:D:536:LEU:HD11	1.93	0.49
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.95	0.49
1:A:76:LEU:HG	1:A:89:ASN:OD1	2.13	0.49
3:D:449:ARG:HB3	3:D:453:GLY:O	2.14	0.48
1:A:191:LEU:HD12	1:A:193:TRP:CG	2.47	0.48
3:D:456:SER:O	3:D:459:GLU:HG2	2.13	0.48
1:A:113:VAL:HG12	1:A:159:ARG:HA	1.96	0.48
2:C:16:ARG:HH12	2:C:92:GLU:CD	2.16	0.48
3:D:492:PHE:O	3:D:493:ASP:C	2.53	0.48
1:A:161:VAL:HB	1:A:162:PRO:HD2	1.93	0.47
2:B:181:CYS:HA	2:B:185:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:ASN:C	2:C:79:GLU:N	2.67	0.47
2:C:178:LYS:N	2:C:179:PRO:CD	2.77	0.47
2:B:125:TRP:N	2:B:125:TRP:CD2	2.82	0.47
2:B:178:LYS:N	2:B:179:PRO:CD	2.77	0.47
1:A:29:SER:OG	1:A:30:VAL:N	2.48	0.47
2:C:107:ASP:HB2	2:C:117:THR:HA	1.97	0.47
2:C:160:THR:HG23	2:C:166:HIS:ND1	2.29	0.47
2:B:151:LEU:HD13	2:B:173:LEU:CB	2.44	0.47
3:D:416:TYR:CD1	3:D:472:LEU:HB3	2.49	0.47
2:B:150:THR:CB	2:B:196:VAL:HG12	2.44	0.47
3:D:434:ILE:HG22	3:D:531:ILE:HG13	1.97	0.47
1:A:82:ASP:HB2	1:A:85:LEU:HD12	1.97	0.46
2:C:52:VAL:CG2	2:C:53:ILE:N	2.77	0.46
2:B:122:PHE:CD2	2:B:172:LEU:HD21	2.51	0.46
2:C:3:ALA:HB1	2:C:37:TYR:CD1	2.50	0.46
2:C:83:ARG:NH1	2:C:83:ARG:HG3	2.29	0.46
2:B:76:PHE:O	2:B:84:SER:HB2	2.14	0.46
2:C:124:LEU:HB3	2:C:126:LYS:O	2.15	0.46
1:A:146:CYS:O	3:D:483:ARG:NH2	2.49	0.46
2:B:150:THR:OG1	2:B:196:VAL:HG12	2.15	0.46
1:A:181:TYR:HA	1:A:223:TYR:O	2.15	0.46
2:B:39:LYS:HG3	2:B:125:TRP:CD1	2.51	0.46
2:C:161:VAL:HB	2:C:163:TRP:CD1	2.51	0.45
3:D:441:TYR:CD2	3:D:460:MET:HG3	2.45	0.45
2:B:135:ILE:CG2	2:B:139:PHE:CE1	3.00	0.45
2:C:34:ILE:CG2	2:C:123:ILE:HD12	2.47	0.45
1:A:96:CYS:O	1:A:100:ILE:HG12	2.16	0.45
1:A:228:TRP:O	1:A:229:ILE:C	2.55	0.45
2:B:76:PHE:O	2:B:84:SER:CB	2.65	0.45
2:B:180:LEU:O	2:B:185:ARG:HA	2.16	0.45
2:B:3:ALA:C	2:B:5:PRO:HD2	2.37	0.45
2:C:11:PRO:N	2:C:12:PRO:CD	2.80	0.45
3:D:415:ILE:O	3:D:418:PHE:N	2.50	0.45
1:A:73:ILE:HG21	1:A:78:LEU:HD21	1.97	0.44
2:B:136:LEU:O	2:B:140:GLU:HB3	2.18	0.44
2:C:90:ILE:HA	2:C:93:ILE:HD12	1.99	0.44
2:C:94:TRP:CD1	2:C:121:TYR:HE2	2.34	0.44
3:D:407:PHE:CE1	3:D:411:ILE:HD11	2.52	0.44
2:C:5:PRO:HG2	2:C:33:ILE:HG12	1.99	0.44
2:B:44:TRP:HB3	2:B:122:PHE:CE1	2.52	0.44
2:C:151:LEU:HD23	2:C:151:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:551:LEU:O	3:D:553:GLY:N	2.50	0.44
2:B:19:ASN:O	2:B:22:THR:N	2.51	0.44
2:B:23:ARG:O	2:B:24:ARG:C	2.56	0.44
2:C:197:ILE:HG22	2:C:198:ALA:N	2.32	0.44
3:D:449:ARG:NH1	3:D:453:GLY:O	2.50	0.44
3:D:532:LEU:HD22	3:D:536:LEU:CD1	2.47	0.44
2:B:161:VAL:HG12	2:B:162:ASN:N	2.33	0.44
2:C:160:THR:HG23	2:C:166:HIS:CD2	2.51	0.44
1:A:89:ASN:HB3	1:A:93:TYR:CZ	2.53	0.43
2:B:25:GLN:O	2:B:26:GLN:C	2.56	0.43
1:A:100:ILE:HD12	3:D:438:VAL:CG1	2.49	0.43
2:B:3:ALA:C	2:B:5:PRO:CD	2.86	0.43
1:A:161:VAL:CB	1:A:162:PRO:CD	2.87	0.43
2:B:106:ILE:HG23	2:B:110:GLY:HA2	1.99	0.43
2:B:124:LEU:HD22	2:B:131:TRP:CE3	2.53	0.43
2:C:38:CYS:HB3	2:C:125:TRP:CH2	2.54	0.43
2:C:154:LEU:O	2:C:159:GLU:HB2	2.17	0.43
2:C:172:LEU:O	2:C:173:LEU:C	2.55	0.43
2:C:131:TRP:HD1	2:C:176:CYS:HG	1.66	0.43
2:C:161:VAL:C	2:C:163:TRP:H	2.22	0.43
1:A:106:THR:HB	1:A:110:ASN:HD21	1.83	0.43
2:C:2:SER:O	2:C:5:PRO:HD3	2.18	0.43
3:D:481:ASN:O	3:D:482:LYS:C	2.56	0.43
1:A:161:VAL:CB	1:A:162:PRO:HD3	2.49	0.43
1:A:181:TYR:HB3	1:A:224:TRP:CD2	2.54	0.43
2:C:16:ARG:CG	2:C:16:ARG:NH1	2.80	0.43
2:C:38:CYS:HB3	2:C:125:TRP:CZ3	2.54	0.43
3:D:408:LEU:O	3:D:409:ASP:C	2.55	0.42
3:D:531:ILE:O	3:D:535:VAL:HG23	2.19	0.42
3:D:546:LEU:HD23	3:D:559:ASN:HB2	2.00	0.42
2:C:1:MET:SD	2:C:4:LEU:HD13	2.60	0.42
2:C:82:GLN:HB2	2:C:83:ARG:H	1.46	0.42
1:A:147:PHE:CD1	1:A:147:PHE:N	2.88	0.42
2:B:39:LYS:HD2	2:B:125:TRP:HB3	2.00	0.42
2:B:36:GLN:HA	2:B:39:LYS:HB3	2.02	0.42
1:A:186:LEU:HD23	1:A:190:ASN:HD21	1.83	0.42
2:B:77:ASN:OD1	2:B:80:ASP:HB3	2.19	0.42
1:A:95:VAL:O	1:A:98:LYS:N	2.53	0.42
2:B:151:LEU:HD13	2:B:173:LEU:HB3	2.01	0.42
1:A:171:LYS:O	1:A:174:GLU:HB2	2.19	0.42
2:B:122:PHE:CD1	2:B:172:LEU:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:HG22	2:B:160:THR:O	2.19	0.42
1:A:41:GLU:O	1:A:44:VAL:HG12	2.20	0.42
1:A:51:ASN:O	1:A:54:LEU:HB3	2.20	0.41
1:A:124:PHE:C	1:A:126:LYS:N	2.73	0.41
1:A:223:TYR:N	1:A:223:TYR:CD2	2.88	0.41
2:B:14:TYR:CE2	2:B:30:TRP:HZ2	2.38	0.41
2:B:104:LEU:HA	2:B:105:PRO:HD3	1.77	0.41
3:D:515:THR:O	3:D:516:GLN:C	2.58	0.41
3:D:551:LEU:HD23	3:D:551:LEU:HA	1.86	0.41
1:A:107:LYS:HG2	1:A:107:LYS:O	2.19	0.41
1:A:140:MET:O	1:A:143:SER:HB2	2.20	0.41
2:B:16:ARG:NH1	2:B:23:ARG:HD3	2.35	0.41
1:A:106:THR:HG21	1:A:114:ILE:HD12	2.02	0.41
3:D:517:ILE:HG23	3:D:518:LEU:N	2.36	0.41
2:B:160:THR:O	2:B:160:THR:CG2	2.68	0.41
2:C:163:TRP:HB3	2:C:165:PHE:CE2	2.56	0.41
2:C:107:ASP:HB3	2:C:117:THR:HG22	2.03	0.41
2:C:189:LEU:HB2	2:C:196:VAL:HG13	2.02	0.41
2:C:16:ARG:NH2	2:C:23:ARG:NH1	2.69	0.41
2:C:94:TRP:HB3	2:C:121:TYR:OH	2.20	0.41
2:C:94:TRP:CH2	2:C:121:TYR:CB	3.04	0.41
2:C:97:MET:HB3	2:C:103:CYS:SG	2.61	0.41
2:B:156:GLU:HG2	2:B:167:ARG:NH1	2.36	0.41
3:D:533:MET:HA	3:D:536:LEU:HD12	2.03	0.41
2:C:25:GLN:OE1	3:D:563:PRO:HG3	2.21	0.40
3:D:524:LYS:HA	3:D:524:LYS:CE	2.51	0.40
2:B:7:VAL:O	2:B:10:PHE:HB3	2.19	0.40
1:A:186:LEU:CD2	1:A:190:ASN:HD21	2.33	0.40
2:B:105:PRO:HB2	2:B:118:THR:HG22	2.04	0.40
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.98	0.40
2:C:3:ALA:HB1	2:C:37:TYR:HD1	1.86	0.40
2:C:179:PRO:O	2:C:183:ARG:HB2	2.21	0.40
1:A:187:LEU:HD12	1:A:198:SER:OG	2.21	0.40
1:A:213:ILE:HD13	1:A:215:TYR:CZ	2.56	0.40
2:B:161:VAL:C	2:B:163:TRP:N	2.75	0.40
3:D:457:PRO:O	3:D:460:MET:N	2.54	0.40
3:D:423:PHE:CG	3:D:424:LYS:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/233 (91%)	188 (89%)	22 (10%)	1 (0%)	29	68
2	B	178/202 (88%)	144 (81%)	28 (16%)	6 (3%)	3	31
2	C	178/202 (88%)	148 (83%)	24 (14%)	6 (3%)	3	31
3	D	169/566 (30%)	145 (86%)	23 (14%)	1 (1%)	25	64
All	All	736/1203 (61%)	625 (85%)	97 (13%)	14 (2%)	8	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	16	ARG
2	C	78	ASN
3	D	563	PRO
2	B	81	ILE
2	B	101	GLY
2	B	162	ASN
2	B	4	LEU
1	A	229	ILE
2	B	99	LYS
2	C	99	LYS
2	B	34	ILE
2	C	178	LYS
2	C	161	VAL
2	C	196	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	195/211 (92%)	149 (76%)	46 (24%)	1 5
2	B	173/192 (90%)	134 (78%)	39 (22%)	1 6
2	C	173/192 (90%)	127 (73%)	46 (27%)	0 3
3	D	160/519 (31%)	117 (73%)	43 (27%)	0 3
All	All	701/1114 (63%)	527 (75%)	174 (25%)	0 4

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	25	LEU
1	A	29	SER
1	A	33	ARG
1	A	41	GLU
1	A	51	ASN
1	A	59	GLU
1	A	60	PHE
1	A	66	HIS
1	A	80	ASP
1	A	81	ARG
1	A	82	ASP
1	A	83	LYS
1	A	84	HIS
1	A	86	PHE
1	A	90	ASP
1	A	91	PHE
1	A	101	GLU
1	A	106	THR
1	A	107	LYS
1	A	119	LEU
1	A	128	ASN
1	A	131	LEU
1	A	139	ASP
1	A	143	SER
1	A	147	PHE
1	A	153	ARG
1	A	158	LEU
1	A	160	SER
1	A	163	ASN
1	A	165	LEU
1	A	166	THR
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	170	THR
1	A	178	ILE
1	A	183	SER
1	A	185	SER
1	A	186	LEU
1	A	191	LEU
1	A	193	TRP
1	A	197	ARG
1	A	200	SER
1	A	210	LEU
1	A	213	ILE
1	A	222	LEU
1	A	232	GLN
2	B	1	MET
2	B	16	ARG
2	B	28	SER
2	B	30	TRP
2	B	36	GLN
2	B	75	LEU
2	B	81	ILE
2	B	83	ARG
2	B	95	SER
2	B	97	MET
2	B	98	THR
2	B	104	LEU
2	B	106	ILE
2	B	107	ASP
2	B	111	ARG
2	B	112	ARG
2	B	113	SER
2	B	114	SER
2	B	117	THR
2	B	120	ARG
2	B	121	TYR
2	B	125	TRP
2	B	129	ASP
2	B	133	SER
2	B	138	TRP
2	B	145	LEU
2	B	151	LEU
2	B	152	TYR
2	B	153	GLU

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Mol	Chain	Res	Type
2	B	154	LEU
2	B	156	GLU
2	B	160	THR
2	B	171	SER
2	B	172	LEU
2	B	181	CYS
2	B	187	THR
2	B	194	ASP
2	B	195	LYS
2	B	197	ILE
2	C	4	LEU
2	C	7	VAL
2	C	16	ARG
2	C	25	GLN
2	C	35	SER
2	C	41	LYS
2	C	42	LYS
2	C	45	TYR
2	C	49	ASP
2	C	51	THR
2	C	52	VAL
2	C	72	SER
2	C	78	ASN
2	C	80	ASP
2	C	81	ILE
2	C	82	GLN
2	C	83	ARG
2	C	85	VAL
2	C	94	TRP
2	C	96	GLN
2	C	97	MET
2	C	107	ASP
2	C	112	ARG
2	C	113	SER
2	C	114	SER
2	C	117	THR
2	C	119	THR
2	C	120	ARG
2	C	121	TYR
2	C	123	ILE
2	C	125	TRP
2	C	127	SER

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Mol	Chain	Res	Type
2	C	128	LEU
2	C	130	SER
2	C	131	TRP
2	C	136	LEU
2	C	138	TRP
2	C	140	GLU
2	C	142	SER
2	C	146	ASN
2	C	152	TYR
2	C	154	LEU
2	C	156	GLU
2	C	171	SER
2	C	182	ASP
2	C	194	ASP
3	D	396	LEU
3	D	398	ARG
3	D	399	GLU
3	D	402	LEU
3	D	403	ASN
3	D	405	GLU
3	D	406	LEU
3	D	421	SER
3	D	430	THR
3	D	432	TYR
3	D	433	MET
3	D	454	LEU
3	D	456	SER
3	D	458	MET
3	D	460	MET
3	D	461	ARG
3	D	462	GLU
3	D	465	GLU
3	D	474	GLU
3	D	476	LYS
3	D	478	VAL
3	D	480	VAL
3	D	482	LYS
3	D	483	ARG
3	D	493	ASP
3	D	498	LYS
3	D	499	LEU
3	D	502	LEU

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Mol	Chain	Res	Type
3	D	506	ASN
3	D	512	LEU
3	D	513	ARG
3	D	514	LEU
3	D	518	LEU
3	D	519	SER
3	D	524	LYS
3	D	531	ILE
3	D	532	LEU
3	D	533	MET
3	D	546	LEU
3	D	547	ILE
3	D	549	LYS
3	D	564	SER
3	D	566	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	51	ASN
1	A	84	HIS
1	A	169	GLN
1	A	190	ASN
1	A	232	GLN
2	B	74	ASN
2	B	96	GLN
2	B	193	ASN
2	C	19	ASN
2	C	26	GLN
2	C	96	GLN
2	C	146	ASN
3	D	403	ASN
3	D	431	ASN
3	D	481	ASN
3	D	538	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 monosaccharides 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	A	213/233 (91%)	0.38	3 (1%)	75	61	57, 60, 61, 62	0
2	B	182/202 (90%)	0.68	24 (13%)	3	2	57, 60, 61, 62	0
2	C	182/202 (90%)	1.03	32 (17%)	1	1	58, 60, 61, 63	0
3	D	171/566 (30%)	0.42	5 (2%)	51	35	57, 59, 61, 62	0
All	All	748/1203 (62%)	0.62	64 (8%)	10	6	57, 60, 61, 63	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	148	VAL	5.7
2	B	164	GLU	4.9
2	C	45	TYR	4.8
2	C	164	GLU	4.6
2	B	42	LYS	4.3
2	C	13	LEU	4.2
2	B	116	THR	4.1
2	C	170	GLU	3.8
2	C	199	ILE	3.8
2	B	148	VAL	3.6
2	B	189	LEU	3.5
2	B	75	LEU	3.4
2	C	183	ARG	3.4
2	C	54	ASN	3.4
2	C	46	MET	3.4
2	C	120	ARG	3.4
2	C	124	LEU	3.3
2	B	43	ILE	3.3
1	A	21	ASN	3.2
2	B	44	TRP	3.1
2	C	141	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	165	PHE	3.1
2	C	52	VAL	3.0
2	C	75	LEU	3.0
2	C	123	ILE	3.0
2	C	145	LEU	2.9
2	C	73	LYS	2.9
2	B	121	TYR	2.9
2	B	165	PHE	2.8
2	C	103	CYS	2.8
2	C	155	SER	2.7
2	C	12	PRO	2.7
2	C	122	PHE	2.7
2	B	45	TYR	2.6
2	C	34	ILE	2.6
2	B	143	GLY	2.5
2	B	78	ASN	2.5
2	C	160	THR	2.4
2	B	155	SER	2.4
1	A	212	TRP	2.3
2	C	93	ILE	2.3
2	C	30	TRP	2.3
2	C	175	TYR	2.3
2	C	146	ASN	2.3
2	B	144	LYS	2.3
1	A	25	LEU	2.3
2	C	53	ILE	2.2
3	D	547	ILE	2.2
2	C	135	ILE	2.2
2	B	123	ILE	2.2
3	D	527	TRP	2.2
3	D	558	LYS	2.1
2	C	87	GLN	2.1
3	D	548	ASP	2.1
2	B	104	LEU	2.1
2	B	162	ASN	2.1
2	B	30	TRP	2.1
3	D	444	TYR	2.1
2	B	76	PHE	2.1
2	B	105	PRO	2.1
2	C	166	HIS	2.0
2	B	195	LYS	2.0
2	B	188	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	8	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 monosaccharides 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.