Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 11:12 PM EST

PDB ID	:	3HFX
Title	:	Crystal structure of carnitine transporter
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Deposited on	:	2009-05-13
Resolution	:	3.15 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 (i)) were used in the production of this report:

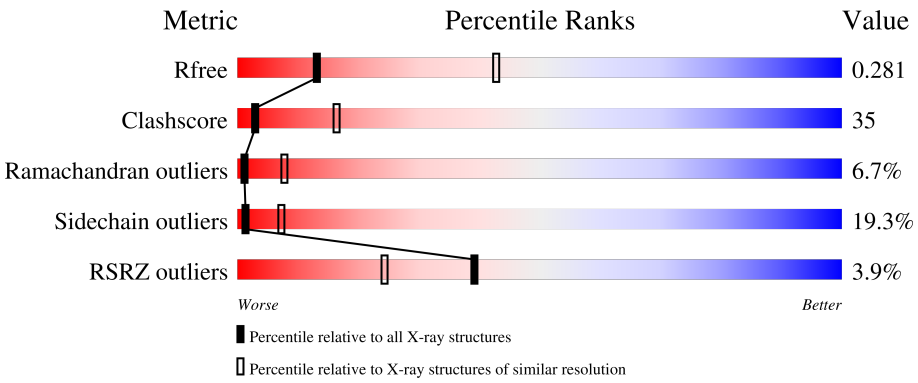
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

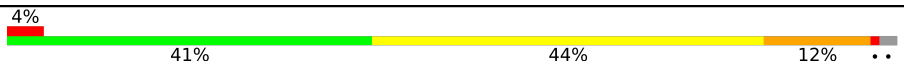
The reported resolution of this entry is 3.15 Å.

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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	504	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HG	A	511	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	152	A	601	-	-	X	-
3	152	A	602	-	-	X	X
3	152	A	603	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3959 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.

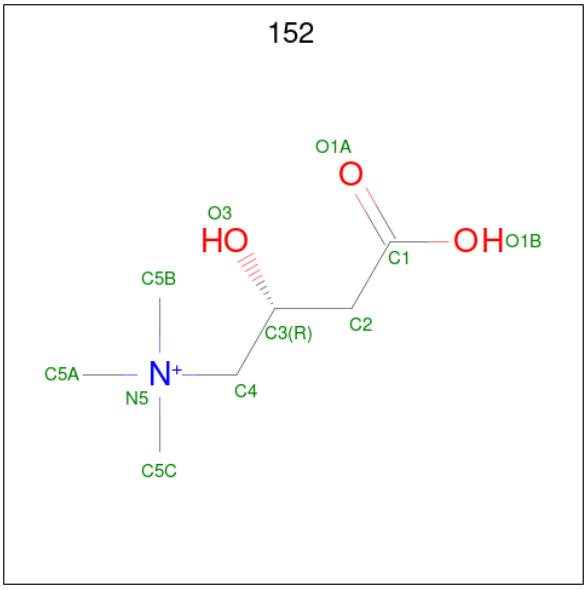
- Molecule 1 is a protein called L-carnitine/gamma-butyrobetaine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	3906	2628	604	646	28	0	0	0

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
2	A	9	9	9	0	0

- Molecule 3 is CARNITINE (three-letter code: 152) (formula: $C_7H_{16}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	7	1	3	0	0
3	A	1	11	7	1	3	0	0

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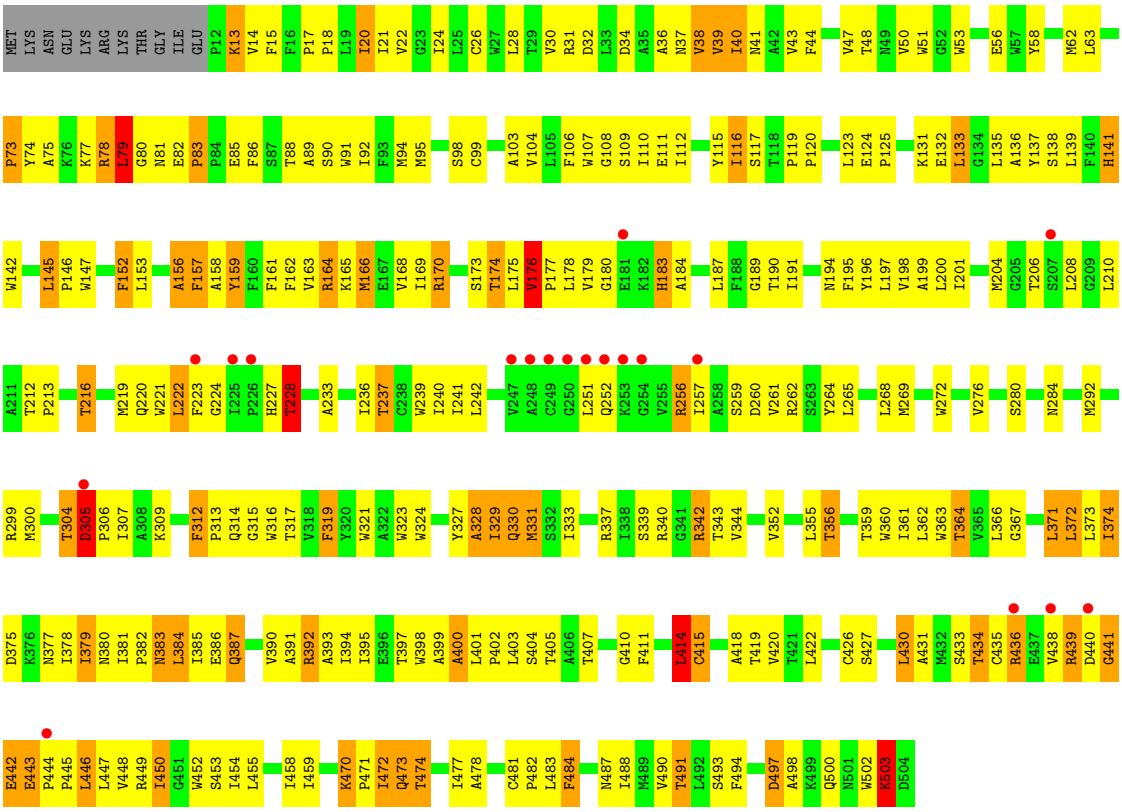
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	7	1	3	0	0
			Total	C	N	O		
3	A	1	11	7	1	3	0	0

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: L-carnitine/gamma-butyrobetaine antiporter

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	134.21Å 134.21Å 85.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.15 39.03 – 3.14	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.15) 99.5 (39.03-3.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.4, CNS 1.0	Depositor
R, R_{free}	0.262 , 0.281 0.261 , 0.281	Depositor DCC
R_{free} test set	1457 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	97.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: 152, HG

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	0.58	0/4033	0.66	4/5514 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	414	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	79	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	305	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	63	LEU	CA-CB-CG	5.07	126.95	115.30

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	3906	0	3963	266	0
2	A	9	0	0	0	0
3	A	44	0	59	30	0
All	All	3959	0	4022	278	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 35.

All (278) 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)
3:A:601:152:C5C	3:A:601:152:H22	1.48	1.41
3:A:601:152:H5C2	3:A:601:152:C2	1.54	1.28
1:A:379:ILE:HG23	1:A:381:ILE:HB	1.40	1.03
1:A:145:LEU:HD22	1:A:145:LEU:H	1.28	0.98
1:A:381:ILE:HG23	1:A:385:ILE:HB	1.44	0.97
1:A:470:LYS:O	1:A:474:THR:HG23	1.65	0.96
1:A:411:PHE:O	1:A:415:CYS:HB2	1.66	0.96
1:A:159:TYR:HE1	1:A:502:TRP:NE1	1.63	0.95
1:A:196:TYR:HA	1:A:483:LEU:HD21	1.52	0.90
1:A:159:TYR:CE1	1:A:502:TRP:NE1	2.36	0.89
1:A:86:PHE:HZ	3:A:604:152:H22	1.35	0.89
1:A:329:ILE:HG13	1:A:330:GLN:N	1.87	0.86
1:A:17:PRO:O	1:A:21:ILE:HG13	1.76	0.84
1:A:86:PHE:CZ	3:A:604:152:H22	2.12	0.84
1:A:201:ILE:HG22	1:A:430:LEU:HD11	1.61	0.83
1:A:327:TYR:CE1	3:A:602:152:H5A1	2.13	0.83
1:A:236:ILE:HA	1:A:239:TRP:CD1	2.15	0.82
1:A:384:LEU:O	1:A:387:GLN:HG2	1.79	0.82
1:A:50:VAL:O	1:A:53:TRP:HZ3	1.61	0.81
1:A:236:ILE:HA	1:A:239:TRP:HD1	1.46	0.81
1:A:199:ALA:HB3	1:A:483:LEU:HD11	1.61	0.80
1:A:381:ILE:CG2	1:A:385:ILE:HB	2.10	0.80
1:A:316:TRP:NE1	3:A:603:152:C5C	2.45	0.80
1:A:487:ASN:O	1:A:491:THR:HG22	1.82	0.79
1:A:194:ASN:O	1:A:198:VAL:HG23	1.83	0.79
1:A:212:THR:OG1	1:A:213:PRO:HD3	1.83	0.79
1:A:447:LEU:HA	1:A:450:ILE:HG12	1.64	0.78
1:A:265:LEU:HD23	1:A:414:LEU:HB2	1.63	0.78
1:A:107:TRP:O	1:A:111:GLU:HB2	1.83	0.78
1:A:379:ILE:HD12	1:A:400:ALA:HB2	1.64	0.78
3:A:601:152:H22	3:A:601:152:H5C2	0.78	0.76
1:A:79:LEU:HD11	1:A:158:ALA:CB	2.16	0.76
1:A:441:GLY:HA2	1:A:445:PRO:HG3	1.66	0.76
1:A:159:TYR:HE1	1:A:502:TRP:HE1	0.87	0.76
1:A:103:ALA:O	1:A:107:TRP:CD1	2.39	0.75
1:A:142:TRP:O	1:A:359:THR:CG2	2.35	0.75
1:A:236:ILE:O	1:A:239:TRP:HB2	1.87	0.74
1:A:79:LEU:HD11	1:A:158:ALA:HB1	1.67	0.74
1:A:142:TRP:O	1:A:359:THR:HG21	1.87	0.74
3:A:601:152:H22	3:A:601:152:H5C3	1.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:O	1:A:53:TRP:CZ3	2.45	0.70
1:A:212:THR:HG21	1:A:236:ILE:CG2	2.22	0.70
1:A:382:PRO:O	1:A:386:GLU:HG2	1.92	0.69
3:A:604:152:O3	3:A:604:152:H5B2	1.92	0.69
1:A:31:ARG:HD2	1:A:32:ASP:HB2	1.73	0.69
1:A:379:ILE:HG22	1:A:379:ILE:O	1.91	0.69
1:A:481:CYS:HB3	1:A:482:PRO:CD	2.23	0.69
1:A:385:ILE:CG2	1:A:393:ALA:HB2	2.23	0.69
1:A:85:GLU:OE1	1:A:340:ARG:HD2	1.92	0.68
1:A:210:LEU:HD21	1:A:472:ILE:HD12	1.75	0.68
1:A:17:PRO:HB2	1:A:18:PRO:HD3	1.75	0.68
1:A:330:GLN:OE1	3:A:602:152:H3	1.93	0.68
1:A:474:THR:HA	1:A:477:ILE:HD12	1.76	0.68
1:A:50:VAL:HG12	1:A:51:TRP:CD1	2.29	0.68
1:A:145:LEU:HD22	1:A:145:LEU:N	2.04	0.67
1:A:443:GLU:HB3	1:A:444:PRO:HD3	1.76	0.66
3:A:602:152:O3	3:A:602:152:H5A2	1.95	0.66
1:A:40:ILE:HD12	1:A:474:THR:HG21	1.77	0.66
1:A:212:THR:HG21	1:A:236:ILE:HG22	1.78	0.66
1:A:312:PHE:HB3	1:A:313:PRO:CD	2.26	0.66
1:A:472:ILE:HG12	1:A:473:GLN:N	2.10	0.65
1:A:116:ILE:CG2	1:A:131:LYS:HA	2.26	0.65
1:A:88:THR:HA	1:A:342:ARG:NH2	2.12	0.65
1:A:473:GLN:O	1:A:477:ILE:HG13	1.96	0.64
1:A:107:TRP:CZ2	1:A:210:LEU:HD11	2.32	0.64
1:A:383:ASN:N	1:A:383:ASN:OD1	2.31	0.63
1:A:360:TRP:O	1:A:364:THR:HG23	1.99	0.63
1:A:379:ILE:C	1:A:381:ILE:H	2.02	0.63
3:A:602:152:O3	3:A:602:152:H5B3	1.99	0.63
1:A:237:THR:HA	1:A:240:ILE:HG12	1.80	0.63
1:A:385:ILE:HG21	1:A:393:ALA:HB2	1.81	0.62
1:A:379:ILE:CG2	1:A:381:ILE:HB	2.24	0.62
1:A:109:SER:OG	1:A:398:TRP:CH2	2.52	0.62
1:A:24:ILE:O	1:A:28:LEU:HB3	2.00	0.62
1:A:20:ILE:O	1:A:24:ILE:HG22	1.99	0.62
1:A:233:ALA:O	1:A:237:THR:HG22	1.99	0.61
1:A:164:ARG:O	1:A:166:MET:N	2.32	0.61
1:A:262:ARG:HG3	1:A:418:ALA:HA	1.83	0.61
1:A:327:TYR:HE1	3:A:602:152:H5A1	1.63	0.61
1:A:312:PHE:O	1:A:315:GLY:N	2.29	0.61
1:A:173:SER:O	1:A:175:LEU:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TRP:CE2	3:A:603:152:C5C	2.85	0.60
1:A:116:ILE:HG21	1:A:131:LYS:HA	1.83	0.59
3:A:601:152:C5C	3:A:601:152:C2	2.30	0.59
1:A:56:GLU:HA	1:A:321:TRP:CZ3	2.37	0.59
1:A:108:GLY:O	1:A:366:LEU:HB3	2.01	0.59
1:A:323:TRP:NE1	1:A:327:TYR:HE2	1.99	0.59
1:A:441:GLY:CA	1:A:445:PRO:HG3	2.33	0.58
1:A:431:ALA:HA	1:A:452:TRP:HZ3	1.69	0.58
1:A:109:SER:HB3	1:A:394:ILE:HG23	1.86	0.58
1:A:204:MET:CE	1:A:426:CYS:HB2	2.34	0.57
1:A:312:PHE:HB3	1:A:313:PRO:HD3	1.87	0.57
1:A:385:ILE:HD11	1:A:392:ARG:HD2	1.86	0.57
1:A:379:ILE:HG12	1:A:381:ILE:HD12	1.87	0.57
1:A:178:LEU:HD13	1:A:497:ASP:HB2	1.86	0.57
1:A:327:TYR:CD2	3:A:601:152:H3	2.41	0.56
1:A:431:ALA:HA	1:A:452:TRP:CZ3	2.41	0.56
1:A:168:VAL:HG11	1:A:175:LEU:HD23	1.87	0.56
1:A:173:SER:C	1:A:175:LEU:H	2.08	0.56
1:A:90:SER:O	1:A:94:MET:HG3	2.05	0.56
1:A:196:TYR:CE2	1:A:200:LEU:HD22	2.41	0.56
1:A:329:ILE:HG13	1:A:330:GLN:H	1.67	0.55
1:A:13:LYS:H	1:A:13:LYS:HD3	1.70	0.55
1:A:156:ALA:HA	1:A:494:PHE:CD1	2.41	0.55
1:A:187:LEU:O	1:A:191:ILE:HG12	2.06	0.55
1:A:22:VAL:HG21	1:A:201:ILE:HD11	1.88	0.55
1:A:142:TRP:O	1:A:359:THR:HG23	2.05	0.54
1:A:304:THR:O	1:A:306:PRO:HD3	2.06	0.54
1:A:305:ASP:H	1:A:314:GLN:HE22	1.55	0.54
1:A:323:TRP:CE2	3:A:601:152:H42	2.43	0.54
1:A:382:PRO:HA	1:A:385:ILE:HG22	1.89	0.54
1:A:112:ILE:HG21	1:A:367:GLY:O	2.07	0.54
1:A:216:THR:O	1:A:219:MET:HB2	2.07	0.54
1:A:379:ILE:O	1:A:379:ILE:CG2	2.56	0.54
1:A:394:ILE:O	1:A:397:THR:HB	2.08	0.54
1:A:147:TRP:CE3	1:A:355:LEU:HD13	2.42	0.54
1:A:135:LEU:CD1	1:A:364:THR:HA	2.37	0.54
3:A:603:152:H5C3	3:A:603:152:O3	2.07	0.54
1:A:14:VAL:HG23	1:A:434:THR:HG23	1.90	0.54
1:A:439:ARG:HH21	1:A:440:ASP:HB3	1.72	0.54
1:A:88:THR:HA	1:A:342:ARG:HH22	1.73	0.53
1:A:56:GLU:HA	1:A:321:TRP:HZ3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TRP:HE1	3:A:603:152:C5C	2.22	0.53
1:A:106:PHE:CE2	1:A:110:ILE:HD11	2.43	0.53
1:A:107:TRP:HZ2	1:A:210:LEU:HD11	1.74	0.53
1:A:257:ILE:O	1:A:261:VAL:HG23	2.09	0.53
1:A:26:CYS:O	1:A:30:VAL:HG23	2.09	0.53
1:A:157:PHE:CZ	1:A:175:LEU:HD21	2.44	0.53
1:A:470:LYS:O	1:A:474:THR:CG2	2.49	0.53
1:A:135:LEU:HD13	1:A:364:THR:HA	1.91	0.52
1:A:146:PRO:HB2	1:A:324:TRP:CZ3	2.44	0.52
1:A:24:ILE:O	1:A:28:LEU:CB	2.57	0.52
1:A:175:LEU:C	1:A:177:PRO:HD3	2.29	0.52
1:A:141:HIS:HE1	1:A:317:THR:OG1	1.92	0.52
1:A:455:LEU:O	1:A:459:ILE:HG13	2.09	0.52
1:A:109:SER:CB	1:A:394:ILE:HG23	2.41	0.51
1:A:219:MET:C	1:A:221:TRP:H	2.14	0.51
1:A:44:PHE:CD2	1:A:477:ILE:CD1	2.93	0.51
1:A:204:MET:SD	1:A:426:CYS:HB2	2.51	0.51
1:A:379:ILE:C	1:A:381:ILE:N	2.64	0.51
1:A:204:MET:HE1	1:A:426:CYS:HB2	1.92	0.51
1:A:272:TRP:HE1	1:A:407:THR:HG21	1.76	0.50
1:A:153:LEU:HD13	1:A:329:ILE:HG22	1.92	0.50
1:A:481:CYS:HB3	1:A:482:PRO:HD2	1.92	0.50
1:A:44:PHE:O	1:A:48:THR:HB	2.12	0.50
1:A:373:LEU:HA	1:A:378:ILE:CG2	2.41	0.50
1:A:227:HIS:O	1:A:228:THR:O	2.29	0.50
1:A:307:ILE:C	1:A:307:ILE:HD12	2.31	0.50
1:A:146:PRO:HB2	1:A:324:TRP:CH2	2.47	0.50
1:A:280:SER:O	1:A:284:ASN:ND2	2.45	0.50
1:A:403:LEU:C	1:A:405:THR:H	2.14	0.49
1:A:161:PHE:HB3	1:A:162:PHE:CE1	2.47	0.49
1:A:316:TRP:CE2	3:A:603:152:H5C2	2.47	0.49
1:A:316:TRP:CZ2	3:A:603:152:H5C1	2.48	0.49
1:A:435:CYS:SG	1:A:436:ARG:N	2.85	0.49
1:A:378:ILE:O	1:A:379:ILE:HG13	2.13	0.49
1:A:272:TRP:HE1	1:A:407:THR:CG2	2.25	0.49
1:A:403:LEU:O	1:A:405:THR:N	2.45	0.49
1:A:175:LEU:HD11	1:A:490:VAL:HG22	1.95	0.48
1:A:276:VAL:HG11	1:A:402:PRO:HD2	1.95	0.48
1:A:179:VAL:HB	1:A:493:SER:HA	1.95	0.48
1:A:206:THR:HG23	1:A:472:ILE:HB	1.94	0.48
1:A:454:ILE:O	1:A:458:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ALA:O	1:A:482:PRO:HD2	2.14	0.48
1:A:89:ALA:HA	1:A:92:ILE:HG12	1.96	0.48
1:A:176:VAL:N	1:A:177:PRO:HD3	2.28	0.48
1:A:117:SER:O	1:A:125:PRO:HB3	2.14	0.48
1:A:434:THR:HB	1:A:452:TRP:HH2	1.78	0.48
1:A:312:PHE:CE1	1:A:316:TRP:CD1	3.02	0.47
1:A:323:TRP:NE1	1:A:327:TYR:CE2	2.80	0.47
1:A:156:ALA:O	1:A:159:TYR:N	2.47	0.47
1:A:152:PHE:HD2	1:A:491:THR:HG1	1.63	0.47
1:A:442:GLU:N	1:A:445:PRO:HG3	2.28	0.47
1:A:184:ALA:O	1:A:189:GLY:HA3	2.13	0.47
1:A:240:ILE:HG22	1:A:453:SER:HB3	1.96	0.47
3:A:604:152:O3	3:A:604:152:H5C3	2.15	0.47
1:A:40:ILE:HG13	1:A:41:ASN:N	2.28	0.47
1:A:173:SER:OG	1:A:184:ALA:HB1	2.14	0.47
1:A:399:ALA:O	1:A:401:LEU:N	2.47	0.47
1:A:481:CYS:HB3	1:A:482:PRO:HD3	1.94	0.47
1:A:115:TYR:OH	1:A:141:HIS:HD2	1.98	0.47
1:A:222:LEU:C	1:A:224:GLY:H	2.17	0.47
1:A:252:GLN:HB2	1:A:256:ARG:HB2	1.97	0.47
1:A:312:PHE:CE1	1:A:316:TRP:HD1	2.33	0.46
1:A:82:GLU:N	1:A:83:PRO:HD3	2.30	0.46
1:A:79:LEU:CD1	1:A:158:ALA:HB1	2.39	0.46
1:A:109:SER:OG	1:A:398:TRP:HH2	1.96	0.46
1:A:133:LEU:HD23	1:A:136:ALA:HB3	1.96	0.46
1:A:103:ALA:O	1:A:107:TRP:HD1	1.98	0.46
1:A:39:VAL:O	1:A:43:VAL:HG13	2.16	0.46
1:A:107:TRP:C	1:A:109:SER:H	2.18	0.46
1:A:381:ILE:O	1:A:382:PRO:C	2.54	0.46
1:A:316:TRP:NE1	3:A:603:152:H5C3	2.30	0.46
1:A:379:ILE:CD1	1:A:400:ALA:HB2	2.42	0.45
3:A:601:152:H5C2	3:A:601:152:H21	1.76	0.45
1:A:141:HIS:CE1	1:A:317:THR:HA	2.52	0.45
1:A:169:ILE:HB	1:A:174:THR:HG21	1.99	0.45
1:A:441:GLY:C	1:A:445:PRO:HG3	2.37	0.45
1:A:502:TRP:HB2	1:A:503:LYS:NZ	2.31	0.45
1:A:316:TRP:CE2	3:A:603:152:H5C1	2.51	0.45
1:A:22:VAL:CG2	1:A:201:ILE:HD11	2.46	0.45
1:A:360:TRP:O	1:A:361:ILE:C	2.55	0.45
1:A:371:LEU:HA	1:A:374:ILE:HG23	1.97	0.45
1:A:398:TRP:CD2	1:A:411:PHE:CE2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ALA:C	1:A:401:LEU:H	2.20	0.45
3:A:601:152:O1B	3:A:601:152:O3	2.30	0.45
1:A:156:ALA:O	1:A:158:ALA:N	2.49	0.45
1:A:58:TYR:CD1	1:A:58:TYR:C	2.89	0.45
1:A:104:VAL:HG23	3:A:601:152:H5C1	1.99	0.44
1:A:157:PHE:CD2	1:A:333:ILE:HG22	2.52	0.44
1:A:386:GLU:OE1	1:A:390:VAL:HG22	2.17	0.44
1:A:446:LEU:H	1:A:448:VAL:HG23	1.82	0.44
1:A:15:PHE:HB2	1:A:434:THR:HG21	2.00	0.44
1:A:28:LEU:HD12	1:A:31:ARG:HE	1.82	0.44
1:A:85:GLU:OE1	1:A:340:ARG:CD	2.63	0.44
1:A:161:PHE:HB3	1:A:162:PHE:CD1	2.53	0.44
1:A:120:PRO:HB3	1:A:312:PHE:CE2	2.53	0.44
1:A:196:TYR:HD2	1:A:197:LEU:HD22	1.82	0.44
1:A:484:PHE:O	1:A:488:ILE:HG23	2.18	0.44
1:A:88:THR:O	1:A:91:TRP:HB3	2.18	0.43
1:A:73:PRO:O	1:A:75:ALA:N	2.51	0.43
1:A:391:ALA:HA	1:A:394:ILE:HD12	2.00	0.43
1:A:414:LEU:O	1:A:418:ALA:HB2	2.18	0.43
1:A:44:PHE:CD1	1:A:44:PHE:C	2.91	0.43
1:A:91:TRP:NE1	1:A:339:SER:OG	2.48	0.43
1:A:390:VAL:HG12	1:A:394:ILE:HD11	2.00	0.43
1:A:145:LEU:H	1:A:145:LEU:CD2	2.02	0.43
1:A:272:TRP:NE1	1:A:407:THR:HG22	2.34	0.43
1:A:440:ASP:CG	1:A:441:GLY:N	2.70	0.43
1:A:17:PRO:HB2	1:A:18:PRO:CD	2.46	0.43
1:A:108:GLY:O	1:A:366:LEU:CB	2.66	0.43
1:A:305:ASP:OD1	1:A:309:LYS:HG2	2.18	0.43
1:A:145:LEU:N	1:A:145:LEU:CD2	2.75	0.43
1:A:323:TRP:CD1	1:A:327:TYR:CE2	3.07	0.43
1:A:116:ILE:HG22	1:A:131:LYS:HA	2.00	0.43
1:A:439:ARG:HB3	1:A:440:ASP:H	1.55	0.43
1:A:22:VAL:HG21	1:A:201:ILE:CD1	2.49	0.42
1:A:352:VAL:O	1:A:356:THR:HB	2.19	0.42
1:A:481:CYS:CB	1:A:482:PRO:CD	2.92	0.42
1:A:132:GLU:O	1:A:292:MET:HE3	2.18	0.42
1:A:36:ALA:C	1:A:38:VAL:H	2.23	0.42
1:A:170:ARG:HB3	1:A:433:SER:HA	2.01	0.42
1:A:443:GLU:CB	1:A:444:PRO:HD3	2.47	0.42
1:A:356:THR:HA	1:A:359:THR:HG22	2.01	0.42
1:A:79:LEU:HD23	1:A:344:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD23	1:A:491:THR:HB	2.01	0.42
1:A:381:ILE:O	1:A:384:LEU:N	2.53	0.42
1:A:470:LYS:N	1:A:471:PRO:CD	2.82	0.42
1:A:79:LEU:HD11	1:A:158:ALA:HB3	1.96	0.42
1:A:414:LEU:O	1:A:414:LEU:HD22	2.18	0.42
1:A:104:VAL:HG22	1:A:363:TRP:CH2	2.55	0.42
1:A:107:TRP:CZ2	1:A:210:LEU:CD1	3.02	0.42
1:A:407:THR:O	1:A:410:GLY:N	2.53	0.42
1:A:47:VAL:HG11	1:A:477:ILE:HG22	2.02	0.41
1:A:159:TYR:C	1:A:161:PHE:H	2.23	0.41
1:A:272:TRP:NE1	1:A:407:THR:CG2	2.83	0.41
1:A:32:ASP:O	1:A:36:ALA:HB2	2.19	0.41
1:A:319:PHE:CG	1:A:473:GLN:HG2	2.55	0.41
1:A:119:PRO:HG2	1:A:123:LEU:O	2.19	0.41
1:A:329:ILE:HD12	1:A:333:ILE:HG23	2.02	0.41
1:A:95:MET:O	1:A:98:SER:OG	2.37	0.41
1:A:173:SER:C	1:A:175:LEU:N	2.74	0.41
1:A:331:MET:HE3	3:A:602:152:H21	2.02	0.41
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.92	0.41
1:A:379:ILE:O	1:A:381:ILE:N	2.42	0.41
1:A:304:THR:HG23	1:A:305:ASP:N	2.36	0.41
1:A:434:THR:CB	1:A:452:TRP:HH2	2.34	0.41
1:A:135:LEU:O	1:A:138:SER:HB2	2.21	0.41
1:A:241:ILE:HG13	1:A:242:LEU:N	2.35	0.41
1:A:316:TRP:NE1	3:A:603:152:H5C2	2.31	0.41
1:A:328:ALA:O	1:A:329:ILE:C	2.59	0.41
1:A:441:GLY:HA2	1:A:445:PRO:CG	2.44	0.41
1:A:147:TRP:CE2	1:A:355:LEU:HB3	2.56	0.41
1:A:312:PHE:O	1:A:313:PRO:C	2.59	0.40
1:A:78:ARG:O	1:A:80:GLY:N	2.51	0.40
1:A:187:LEU:HG	1:A:191:ILE:HD13	2.02	0.40
1:A:304:THR:O	1:A:306:PRO:CD	2.69	0.40
1:A:316:TRP:NE1	3:A:603:152:H5C1	2.34	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	491/504 (97%)	372 (76%)	86 (18%)	33 (7%)	1 8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	PRO
1	A	156	ALA
1	A	165	LYS
1	A	174	THR
1	A	228	THR
1	A	400	ALA
1	A	404	SER
1	A	438	VAL
1	A	78	ARG
1	A	141	HIS
1	A	157	PHE
1	A	328	ALA
1	A	441	GLY
1	A	442	GLU
1	A	503	LYS
1	A	37	ASN
1	A	81	ASN
1	A	183	HIS
1	A	223	PHE
1	A	380	ASN
1	A	497	ASP
1	A	180	GLY
1	A	222	LEU
1	A	375	ASP
1	A	79	LEU
1	A	176	VAL
1	A	377	ASN
1	A	379	ILE

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Mol	Chain	Res	Type
1	A	498	ALA
1	A	220	GLN
1	A	305	ASP
1	A	83	PRO
1	A	312	PHE

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	415/425 (98%)	335 (81%)	80 (19%)	1 7

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	20	ILE
1	A	34	ASP
1	A	38	VAL
1	A	39	VAL
1	A	40	ILE
1	A	62	MET
1	A	74	TYR
1	A	77	LYS
1	A	99	CYS
1	A	116	ILE
1	A	124	GLU
1	A	133	LEU
1	A	137	TYR
1	A	139	LEU
1	A	145	LEU
1	A	152	PHE
1	A	159	TYR
1	A	163	VAL
1	A	164	ARG
1	A	166	MET

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	176	VAL
1	A	183	HIS
1	A	190	THR
1	A	195	PHE
1	A	208	LEU
1	A	216	THR
1	A	228	THR
1	A	237	THR
1	A	251	LEU
1	A	256	ARG
1	A	259	SER
1	A	260	ASP
1	A	264	TYR
1	A	268	LEU
1	A	269	MET
1	A	299	ARG
1	A	300	MET
1	A	304	THR
1	A	319	PHE
1	A	329	ILE
1	A	330	GLN
1	A	331	MET
1	A	337	ARG
1	A	342	ARG
1	A	343	THR
1	A	356	THR
1	A	362	LEU
1	A	364	THR
1	A	371	LEU
1	A	372	LEU
1	A	374	ILE
1	A	383	ASN
1	A	384	LEU
1	A	387	GLN
1	A	392	ARG
1	A	395	ILE
1	A	414	LEU
1	A	415	CYS
1	A	419	THR
1	A	420	VAL
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	427	SER
1	A	430	LEU
1	A	434	THR
1	A	436	ARG
1	A	439	ARG
1	A	443	GLU
1	A	446	LEU
1	A	449	ARG
1	A	450	ILE
1	A	470	LYS
1	A	472	ILE
1	A	473	GLN
1	A	474	THR
1	A	484	PHE
1	A	491	THR
1	A	500	GLN
1	A	503	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	49	ASN
1	A	141	HIS
1	A	473	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	152	A	604	-	10,10,10	1.34	1 (10%)	14,14,14	1.23	2 (14%)
3	152	A	603	-	10,10,10	1.20	1 (10%)	14,14,14	1.38	1 (7%)
3	152	A	601	-	10,10,10	1.48	1 (10%)	14,14,14	1.31	1 (7%)
3	152	A	602	-	10,10,10	1.33	1 (10%)	14,14,14	1.20	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	152	A	604	-	-	8/9/9/9	-
3	152	A	603	-	-	2/9/9/9	-
3	152	A	601	-	-	7/9/9/9	-
3	152	A	602	-	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	152	C4-N5	-2.83	1.46	1.52
3	A	602	152	C4-N5	-2.70	1.46	1.52
3	A	601	152	C4-N5	-2.69	1.46	1.52
3	A	603	152	C4-N5	-2.35	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	152	C3-C4-N5	-4.29	109.48	116.83
3	A	601	152	C4-C3-C2	3.69	114.79	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	152	C3-C4-N5	-3.46	110.92	116.83
3	A	602	152	C3-C4-N5	-3.03	111.65	116.83
3	A	604	152	C3-C2-C1	-2.33	108.29	112.97

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	152	C2-C3-C4-N5
3	A	601	152	O3-C3-C4-N5
3	A	603	152	C1-C2-C3-O3
3	A	603	152	C1-C2-C3-C4
3	A	604	152	C1-C2-C3-O3
3	A	604	152	C1-C2-C3-C4
3	A	601	152	C3-C4-N5-C5C
3	A	601	152	C3-C4-N5-C5A
3	A	601	152	C3-C4-N5-C5B
3	A	602	152	O3-C3-C4-N5
3	A	604	152	O3-C3-C4-N5
3	A	601	152	C1-C2-C3-O3
3	A	601	152	C1-C2-C3-C4
3	A	602	152	O1B-C1-C2-C3
3	A	604	152	O1B-C1-C2-C3
3	A	602	152	O1A-C1-C2-C3
3	A	604	152	O1A-C1-C2-C3
3	A	604	152	C3-C4-N5-C5A
3	A	604	152	C3-C4-N5-C5B
3	A	604	152	C3-C4-N5-C5C

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	152	4	0
3	A	603	152	10	0
3	A	601	152	10	0
3	A	602	152	6	0

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	493/504 (97%)	0.08	19 (3%) 39 24	35, 64, 93, 104	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	GLY	4.6
1	A	253	LYS	4.2
1	A	181	GLU	4.0
1	A	444	PRO	4.0
1	A	254	GLY	3.8
1	A	305	ASP	3.4
1	A	438	VAL	3.4
1	A	247	VAL	3.4
1	A	251	LEU	3.3
1	A	248	ALA	3.2
1	A	252	GLN	3.2
1	A	207	SER	3.0
1	A	225	ILE	2.8
1	A	249	CYS	2.6
1	A	226	PRO	2.4
1	A	257	ILE	2.3
1	A	440	ASP	2.2
1	A	223	PHE	2.2
1	A	436	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	152	A	604	11/11	0.68	0.37	61,62,63,63	0
2	HG	A	511	1/1	0.72	1.06	75,75,75,75	1
2	HG	A	512	1/1	0.73	0.15	83,83,83,83	1
2	HG	A	513	1/1	0.75	0.10	88,88,88,88	1
3	152	A	602	11/11	0.80	0.50	61,62,62,63	0
3	152	A	603	11/11	0.82	0.32	60,60,61,61	0
3	152	A	601	11/11	0.88	0.46	50,52,53,53	0
2	HG	A	505	1/1	0.90	0.10	79,79,79,79	1
2	HG	A	508	1/1	0.91	0.05	104,104,104,104	1
2	HG	A	509	1/1	0.92	0.16	77,77,77,77	1
2	HG	A	510	1/1	0.94	0.21	79,79,79,79	1
2	HG	A	507	1/1	0.97	0.09	96,96,96,96	1
2	HG	A	506	1/1	0.98	0.15	74,74,74,74	1

6.5 Other polymers (i)

There are no such residues in this entry.