Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:05 PM GMT

PDB ID	:	1NDI
Title	:	Carnitine Acetyltransferase in complex with CoA
Authors	:	Jogl, G.; Tong, L.
Deposited on	:	2002-12-09
Resolution	:	2.30 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
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)	:	trunk26865

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 2.30 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	Percentile Ranks	Value
Rfree		0.356
Clashscore		29
Ramachandran outliers		1.9%
Sidechain outliers		5.0%
RSRZ outliers		3.4%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
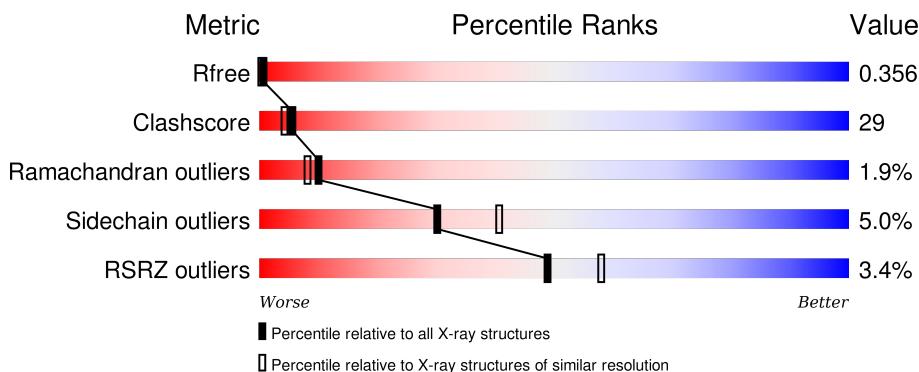
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	A	596	4% — 49% / 46% / •
1	B	596	2% — 51% / 46% / •
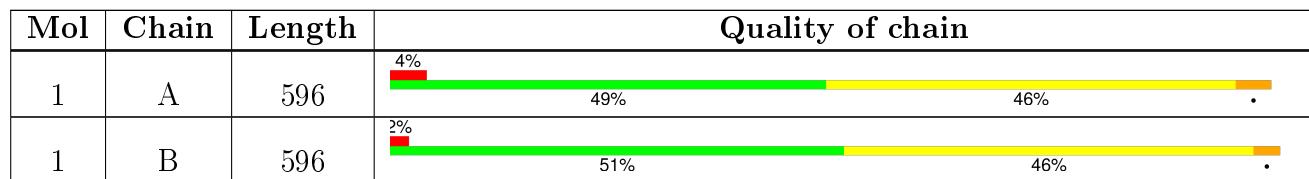
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10303 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 Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total 4757	C 3034	N 820	O 875	S 28	0	0	0
1	B	596	Total 4757	C 3034	N 820	O 875	S 28	0	0	0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
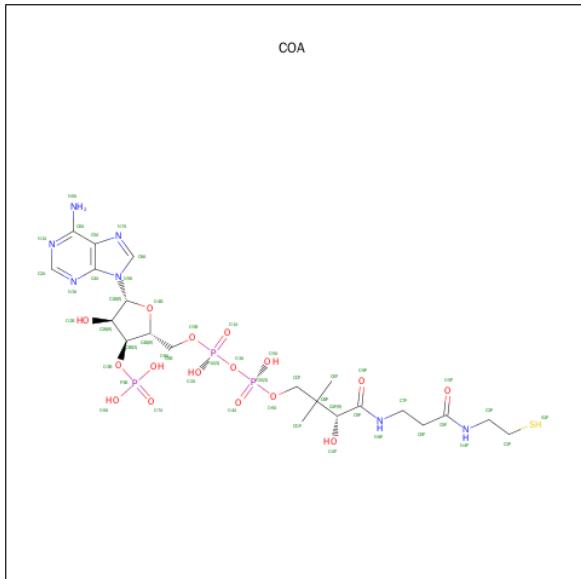
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	342	Total　O 342　　342	0	0
3	B	351	Total　O 351　　351	0	0

3 Residue-property plots ⓘ

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: Carnitine Acetyltransferase

- Molecule 1: Carnitine Acetyltransferase
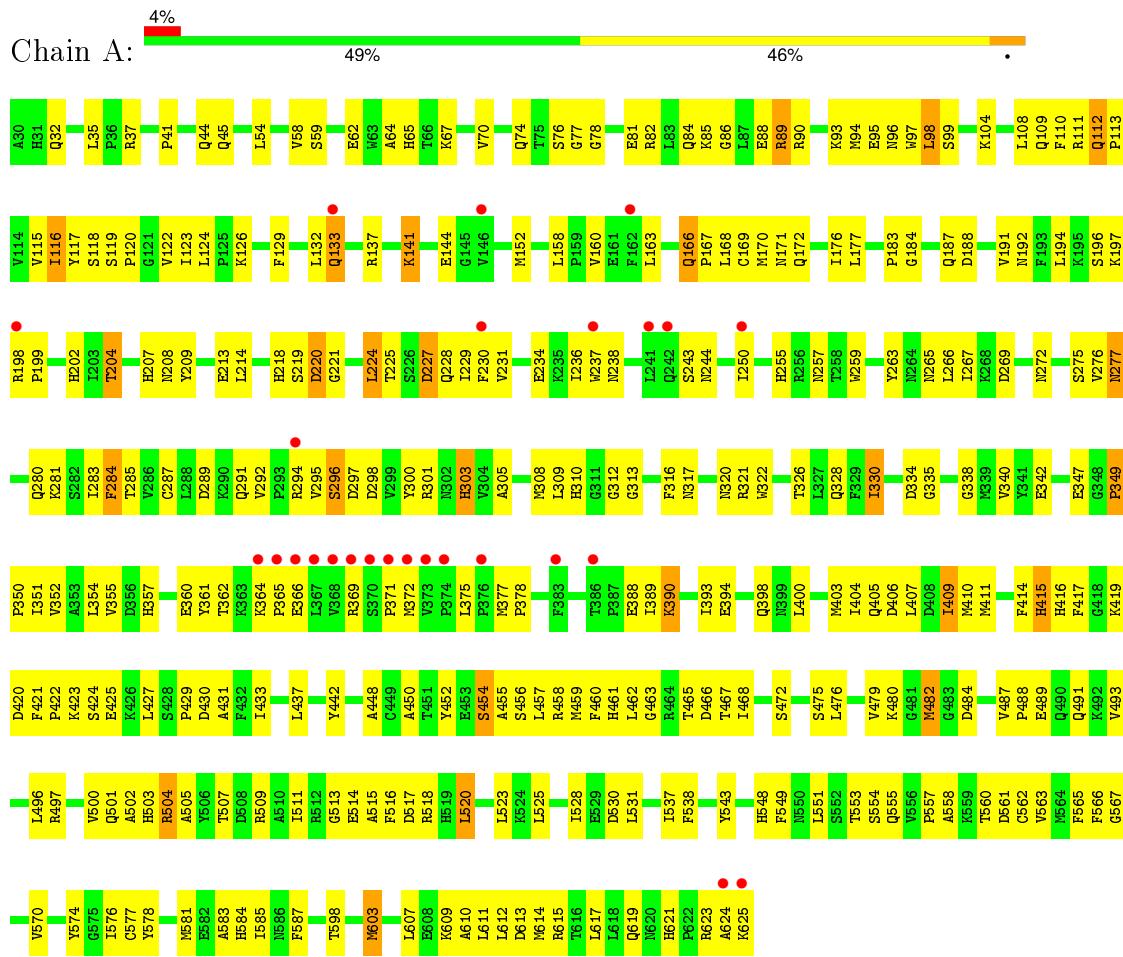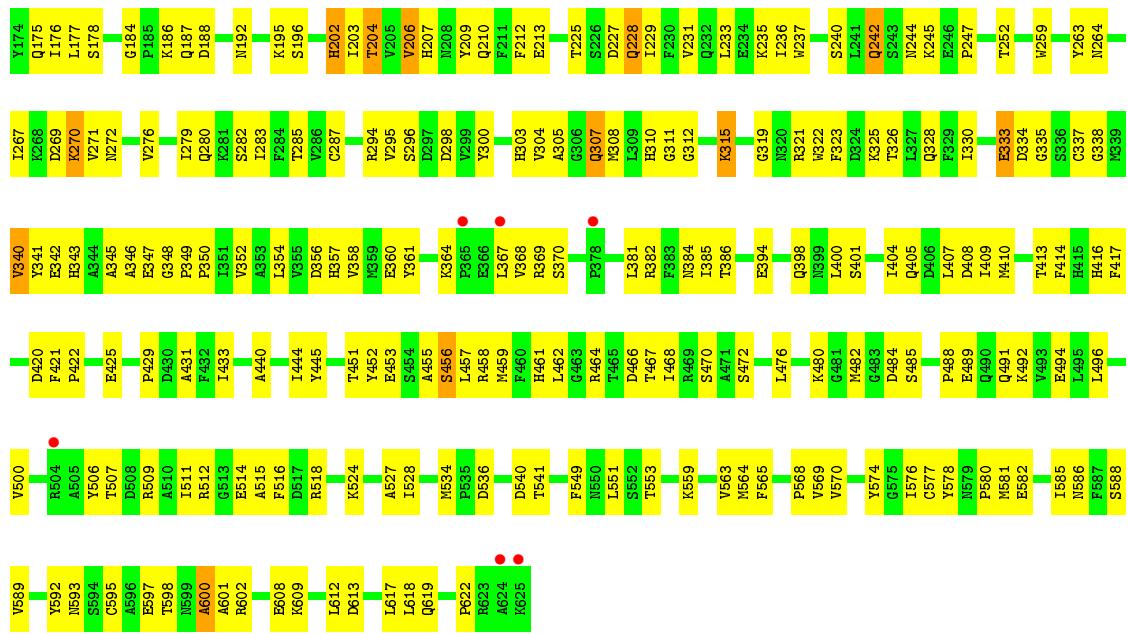
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.26Å　　92.05Å　　122.90Å 90.00°　　128.98°　　90.00°	Depositor
Resolution (Å)	30.00　–　2.30 29.75　–　2.28	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-2.30) 76.0 (29.75-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270　,　0.363 0.271　,　0.356	Depositor DCC
R_{free} test set	4090 reflections (7.66%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.4	EDS
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Outliers	0 of 56477 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10303	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 (i)

5.1 Standard geometry (i)

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

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	0.44	0/4872	0.63	0/6600
1	B	0.47	0/4872	0.64	0/6600
All	All	0.46	0/9744	0.64	0/13200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4733	279	0
1	B	4757	0	4733	281	0
2	A	48	0	32	5	0
2	B	48	0	32	7	0
3	A	342	0	0	31	0
3	B	351	0	0	52	0
All	All	10303	0	9530	563	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 29.

All (563) 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:B:410:MET:HG2	1:B:601:ALA:HA	1.36	1.05
1:B:585:ILE:HG22	3:B:6421:HOH:O	1.60	1.02
1:A:90:ARG:HD3	1:A:97:TRP:HB2	1.44	0.98
1:A:32:GLN:HE22	1:A:170:MET:H	1.15	0.93
1:A:310:HIS:HD2	1:A:312:GLY:H	1.15	0.90
1:B:132:LEU:H	1:B:132:LEU:HD22	1.37	0.89
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.56	0.88
1:A:287:CYS:HB2	1:A:330:ILE:HG22	1.57	0.86
1:B:398:GLN:HB2	3:B:6312:HOH:O	1.75	0.84
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.58	0.84
1:B:330:ILE:HG23	3:B:6202:HOH:O	1.77	0.82
1:B:150:LYS:HE3	1:B:283:ILE:HG12	1.61	0.82
1:B:202:HIS:ND1	1:B:213:GLU:HG3	1.95	0.81
1:B:348:GLY:H	2:B:6170:COA:H32	1.47	0.79
1:A:414:PHE:CE1	1:A:416:HIS:HD2	1.99	0.79
1:B:96:ASN:HB3	1:B:99:SER:OG	1.81	0.79
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.65	0.79
1:A:450:ALA:HB3	1:A:548:HIS:O	1.84	0.78
1:B:451:THR:HG23	1:B:551:LEU:HB3	1.66	0.77
1:B:431:ALA:HB2	3:B:6348:HOH:O	1.85	0.76
1:B:90:ARG:NE	1:B:94:MET:HE1	2.00	0.76
1:B:315:LYS:H	1:B:315:LYS:HD3	1.51	0.76
1:B:410:MET:HB2	3:B:6384:HOH:O	1.85	0.76
1:A:85:LYS:HG3	1:A:89:ARG:HH12	1.52	0.75
1:A:398:GLN:HG3	3:A:5300:HOH:O	1.88	0.74
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.24	0.72
1:B:47:LEU:HD13	1:B:74:GLN:HB3	1.70	0.72
1:B:120:PRO:HB2	1:B:341:TYR:HE2	1.52	0.72
1:A:520:LEU:HD13	1:A:538:PHE:HE2	1.54	0.72
1:B:553:THR:HG22	1:B:576:ILE:HB	1.71	0.72
1:A:309:LEU:HB2	1:A:565:PHE:HE1	1.55	0.71
1:B:177:LEU:HD22	1:B:283:ILE:HG22	1.72	0.71
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.72	0.71
1:B:410:MET:HE2	3:B:6334:HOH:O	1.91	0.71
1:A:141:LYS:HD2	1:A:362:THR:HA	1.73	0.70
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.26	0.70
1:B:242:GLN:HG3	1:B:245:LYS:HE2	1.72	0.70
1:B:204:THR:HG21	1:B:279:ILE:HG12	1.72	0.70
1:B:602:ARG:HD3	3:B:6287:HOH:O	1.92	0.70
1:B:410:MET:HG2	1:B:601:ALA:CA	2.19	0.69
1:B:150:LYS:HD2	1:B:283:ILE:HG21	1.75	0.69

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:HA3	3:A:5189:HOH:O	1.93	0.69
1:A:511:ILE:HD11	2:A:5170:COA:H143	1.72	0.69
1:B:394:GLU:O	1:B:398:GLN:HG3	1.92	0.69
1:A:171:ASN:HB2	3:A:5235:HOH:O	1.92	0.69
1:A:204:THR:HB	1:A:285:THR:HG23	1.73	0.69
1:B:340:VAL:HB	3:B:6174:HOH:O	1.92	0.69
1:B:166:GLN:HG2	3:B:6183:HOH:O	1.92	0.69
1:B:361:TYR:HA	1:B:364:LYS:HD2	1.75	0.69
1:B:161:GLU:H	1:B:170:MET:HE3	1.58	0.68
1:B:120:PRO:HB2	1:B:341:TYR:CE2	2.29	0.68
1:B:225:THR:H	1:B:228:GLN:NE2	1.92	0.68
1:B:171:ASN:ND2	1:B:175:GLN:HE21	1.92	0.67
1:B:322:TRP:H	1:B:328:GLN:NE2	1.93	0.67
1:A:225:THR:H	1:A:228:GLN:NE2	1.92	0.67
1:A:110:PHE:CE2	1:A:112:GLN:HB2	2.30	0.67
1:B:509:ARG:HB3	1:B:514:GLU:HB2	1.76	0.67
1:B:142:LEU:O	1:B:146:VAL:HG23	1.95	0.67
1:A:163:LEU:HB2	1:A:168:LEU:HD21	1.77	0.67
1:B:578:TYR:HB2	3:B:6421:HOH:O	1.94	0.66
1:B:609:LYS:NZ	1:B:613:ASP:OD1	2.28	0.66
1:A:202:HIS:O	1:A:283:ILE:HG13	1.96	0.66
1:B:213:GLU:HB2	1:B:381:LEU:HD21	1.76	0.66
2:B:6170:COA:H141	2:B:6170:COA:O9P	1.95	0.66
1:B:98:LEU:HD21	1:B:518:ARG:HD2	1.77	0.66
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.77	0.66
1:A:295:VAL:HG12	1:A:296:SER:H	1.60	0.66
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.76	0.66
1:B:143:ILE:HG13	3:B:6342:HOH:O	1.95	0.65
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.32	0.65
1:B:225:THR:H	1:B:228:GLN:HE21	1.43	0.65
1:B:601:ALA:HB2	3:B:6384:HOH:O	1.96	0.65
1:A:525:LEU:HD23	1:A:528:ILE:HD12	1.79	0.64
1:B:459:MET:HG2	3:B:6375:HOH:O	1.96	0.64
1:A:54:LEU:O	1:A:58:VAL:HG22	1.98	0.64
1:A:390:LYS:O	1:A:394:GLU:HG2	1.97	0.63
1:B:577:CYS:N	3:B:6224:HOH:O	2.32	0.63
1:A:310:HIS:CD2	1:A:312:GLY:H	2.07	0.63
1:B:476:LEU:HG	1:B:480:LYS:HE3	1.79	0.63
1:B:247:PRO:HB2	1:B:319:GLY:HA3	1.79	0.63
1:B:326:THR:HA	1:B:342:GLU:HB2	1.81	0.62
1:A:584:HIS:C	1:A:585:ILE:HG13	2.20	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.64	0.62
1:B:308:MET:C	3:B:6174:HOH:O	2.37	0.62
1:A:390:LYS:NZ	1:A:390:LYS:HB2	2.15	0.62
1:A:198:ARG:HH12	1:A:281:LYS:NZ	1.97	0.62
1:B:440:ALA:O	1:B:444:ILE:HG13	1.99	0.61
1:B:271:VAL:HG22	3:B:6326:HOH:O	1.99	0.61
1:B:75:THR:O	1:B:81:GLU:HG3	2.01	0.61
1:B:178:SER:HA	1:B:282:SER:O	1.99	0.61
1:B:202:HIS:O	1:B:283:ILE:HD12	1.99	0.61
1:B:94:MET:SD	3:B:6210:HOH:O	2.56	0.61
1:B:124:LEU:HB2	1:B:337:CYS:SG	2.41	0.61
1:A:85:LYS:CG	1:A:89:ARG:HH12	2.14	0.61
1:A:389:ILE:O	1:A:393:ILE:HG13	2.01	0.61
1:B:206:VAL:HA	1:B:210:GLN:O	2.01	0.61
1:A:152:MET:HB3	1:A:158:LEU:HD12	1.82	0.61
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.65	0.61
1:A:420:ASP:OD2	1:A:583:ALA:HA	2.01	0.61
1:A:44:GLN:HB3	3:A:5195:HOH:O	2.02	0.60
1:B:322:TRP:H	1:B:328:GLN:HE22	1.48	0.60
1:A:421:PHE:CE1	1:A:615:ARG:HG3	2.36	0.60
1:B:276:VAL:O	1:B:280:GLN:HG3	2.01	0.60
1:A:482:MET:HE1	1:A:617:LEU:HD22	1.83	0.60
1:A:32:GLN:NE2	1:A:170:MET:H	1.95	0.59
1:B:354:LEU:O	1:B:358:VAL:HG23	2.02	0.59
1:A:218:HIS:C	1:A:220:ASP:H	2.05	0.59
1:A:515:ALA:HB1	3:A:5426:HOH:O	2.01	0.59
1:A:184:GLY:HA3	1:A:187:GLN:O	2.03	0.59
1:A:612:LEU:HD23	1:A:615:ARG:HH21	1.67	0.59
1:A:349:PRO:HB2	1:A:350:PRO:CD	2.31	0.58
1:B:104:LYS:O	1:B:109:GLN:HB2	2.03	0.58
1:A:54:LEU:HD22	1:A:58:VAL:HG11	1.86	0.58
1:B:524:LYS:HG3	1:B:534:MET:SD	2.43	0.58
1:B:400:LEU:O	1:B:404:ILE:HG13	2.03	0.58
1:B:133:GLN:HG3	1:B:134:GLY:N	2.17	0.58
1:A:214:LEU:HB2	1:A:236:ILE:HD11	1.85	0.58
1:A:557:PRO:HB3	3:A:5430:HOH:O	2.03	0.58
1:B:242:GLN:HB2	1:B:244:ASN:OD1	2.04	0.58
1:A:297:ASP:HA	1:A:300:TYR:HB2	1.86	0.58
1:B:431:ALA:CB	1:B:500:VAL:HG13	2.34	0.58
1:A:463:GLY:HA2	3:A:5332:HOH:O	2.04	0.57
1:A:59:SER:HB3	1:A:62:GLU:HG3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:O	1:A:88:GLU:HG3	2.04	0.57
1:B:407:LEU:HD12	1:B:408:ASP:H	1.69	0.57
1:A:461:HIS:CD2	1:A:462:LEU:HG	2.39	0.57
1:A:598:THR:HG21	3:A:5233:HOH:O	2.03	0.57
1:A:610:ALA:O	1:A:614:MET:HG3	2.04	0.57
1:B:414:PHE:CE1	1:B:608:GLU:HG3	2.40	0.57
1:A:194:LEU:HD22	3:A:5207:HOH:O	2.05	0.57
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.40	0.57
1:A:489:GLU:O	1:A:493:VAL:HG23	2.05	0.57
1:A:530:ASP:O	1:A:531:LEU:HB2	2.04	0.57
1:B:461:HIS:CE1	1:B:462:LEU:HD12	2.40	0.57
2:B:6170:COA:O2A	2:B:6170:COA:H8A	2.05	0.56
1:A:615:ARG:HG2	1:A:619:GLN:NE2	2.20	0.56
1:B:76:SER:C	1:B:78:GLY:H	2.08	0.56
1:A:454:SER:HB2	1:A:554:SER:HB3	1.87	0.56
1:A:455:ALA:HB2	1:A:468:ILE:CD1	2.35	0.56
1:B:488:PRO:HB3	3:B:6240:HOH:O	2.05	0.56
1:A:472:SER:H	1:A:475:SER:HB3	1.70	0.56
1:B:132:LEU:HD12	1:B:237:TRP:CZ2	2.40	0.56
1:A:501:GLN:HE22	1:A:504:ARG:HD3	1.70	0.56
1:A:78:GLY:HA2	3:A:5240:HOH:O	2.04	0.56
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.70	0.56
1:B:160:VAL:HG23	3:B:6483:HOH:O	2.06	0.56
1:B:172:GLN:OE1	1:B:346:ALA:HB1	2.05	0.56
1:A:561:ASP:HA	1:A:581:MET:HE1	1.88	0.56
1:B:595:CYS:SG	1:B:598:THR:HG23	2.46	0.55
1:A:98:LEU:O	1:A:98:LEU:HD12	2.05	0.55
1:A:218:HIS:HB2	1:A:220:ASP:OD1	2.07	0.55
1:B:414:PHE:HE1	1:B:608:GLU:HG3	1.71	0.55
1:B:295:VAL:HG11	1:B:303:HIS:CD2	2.42	0.55
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.87	0.55
1:A:561:ASP:OD1	1:A:581:MET:HE2	2.06	0.55
1:B:195:LYS:HB3	3:B:6260:HOH:O	2.06	0.55
1:B:512:ARG:HH11	1:B:512:ARG:HG3	1.70	0.55
1:B:242:GLN:HG3	1:B:245:LYS:CE	2.37	0.55
1:A:351:ILE:O	1:A:355:VAL:HG23	2.06	0.55
1:B:126:LYS:NZ	1:B:334:ASP:O	2.35	0.55
1:B:122:VAL:HG22	1:B:564:MET:HG3	1.88	0.55
1:A:431:ALA:HA	1:A:503:HIS:CE1	2.41	0.55
1:B:482:MET:HA	1:B:492:LYS:HD3	1.89	0.55
1:B:43:LEU:HD13	1:B:84:GLN:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:O	1:B:235:LYS:HG3	2.06	0.55
1:A:85:LYS:HG3	1:A:89:ARG:NH1	2.20	0.54
1:A:122:VAL:O	1:A:308:MET:HG2	2.06	0.54
1:A:227:ASP:HA	3:A:5205:HOH:O	2.06	0.54
1:A:250:ILE:HD11	1:A:400:LEU:HD23	1.90	0.54
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.43	0.54
1:B:321:ARG:HH21	1:B:330:ILE:HD13	1.72	0.54
1:B:578:TYR:HD2	1:B:580:PRO:HG3	1.73	0.54
1:B:143:ILE:O	1:B:147:LEU:HG	2.07	0.53
1:A:501:GLN:NE2	1:A:504:ARG:HD3	2.23	0.53
1:B:176:ILE:HA	1:B:326:THR:HG21	1.90	0.53
1:A:537:ILE:HG23	1:A:538:PHE:N	2.22	0.53
1:B:171:ASN:ND2	1:B:175:GLN:NE2	2.56	0.53
1:A:560:THR:HB	3:A:5321:HOH:O	2.08	0.53
1:A:313:GLY:H	1:A:404:ILE:HD13	1.72	0.53
1:B:89:ARG:HB3	3:B:6356:HOH:O	2.09	0.53
1:B:173:TYR:OH	1:B:350:PRO:HA	2.07	0.53
1:B:401:SER:O	1:B:405:GLN:HG3	2.08	0.53
1:B:99:SER:HB2	3:B:6250:HOH:O	2.08	0.53
1:B:576:ILE:HG12	1:B:589:VAL:HG22	1.91	0.53
1:A:461:HIS:NE2	1:A:462:LEU:HG	2.23	0.53
1:A:90:ARG:NE	1:A:97:TRP:O	2.40	0.52
1:B:270:LYS:HG3	1:B:271:VAL:N	2.24	0.52
1:A:496:LEU:HD12	1:A:617:LEU:HD23	1.92	0.52
1:B:31:HIS:HA	3:B:6320:HOH:O	2.09	0.52
1:A:482:MET:HA	1:A:482:MET:HE2	1.90	0.52
1:B:321:ARG:NH2	1:B:330:ILE:HD13	2.24	0.52
1:B:166:GLN:HB3	1:B:459:MET:HE2	1.91	0.52
1:B:272:ASN:O	1:B:276:VAL:HG23	2.09	0.52
1:B:269:ASP:OD2	1:B:384:ASN:ND2	2.41	0.52
1:A:45:GLN:HE22	1:A:514:GLU:HG2	1.75	0.52
1:A:476:LEU:HD11	1:A:480:LYS:HE3	1.91	0.52
1:B:46:SER:HB3	1:B:516:PHE:HB2	1.92	0.52
2:B:6170:COA:H132	3:B:6354:HOH:O	2.08	0.52
1:A:113:PRO:HB2	1:A:403:MET:HE3	1.92	0.52
1:A:448:ALA:HB2	1:A:476:LEU:HD13	1.92	0.52
1:B:296:SER:HB3	1:B:298:ASP:OD1	2.10	0.52
1:A:96:ASN:HB3	1:A:99:SER:OG	2.09	0.52
1:A:466:ASP:OD1	1:A:518:ARG:HG2	2.09	0.52
1:B:133:GLN:HG3	1:B:134:GLY:H	1.75	0.52
1:A:615:ARG:O	1:A:619:GLN:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:HIS:O	1:A:360:GLU:HB3	2.10	0.52
1:B:138:PHE:C	1:B:140:ALA:H	2.13	0.52
1:A:554:SER:HB2	2:A:5170:COA:H22	1.92	0.52
1:A:228:GLN:HG2	1:A:375:LEU:HD11	1.92	0.52
1:A:104:LYS:HE3	1:A:187:GLN:HE22	1.74	0.52
1:A:124:LEU:HG	1:A:338:GLY:HA2	1.92	0.52
1:A:84:GLN:NE2	1:A:523:LEU:HD21	2.25	0.51
1:B:413:THR:N	3:B:6204:HOH:O	2.43	0.51
1:B:171:ASN:HD21	1:B:175:GLN:NE2	2.08	0.51
1:B:540:ASP:OD2	1:B:541:THR:N	2.44	0.51
1:A:255:HIS:CD2	1:A:257:ASN:H	2.28	0.51
1:B:94:MET:CE	1:B:97:TRP:HA	2.40	0.51
1:A:430:ASP:HB2	1:A:555:GLN:NE2	2.25	0.51
1:A:41:PRO:HG3	1:A:513:GLY:O	2.10	0.51
1:A:287:CYS:HB3	1:A:320:ASN:HD22	1.75	0.51
1:A:390:LYS:HZ2	1:A:390:LYS:HB2	1.76	0.51
1:A:276:VAL:O	1:A:280:GLN:HG3	2.10	0.51
1:B:212:PHE:CD1	1:B:236:ILE:HG23	2.46	0.51
1:A:227:ASP:O	1:A:231:VAL:HG23	2.10	0.51
1:A:202:HIS:ND1	1:A:213:GLU:HG3	2.25	0.51
1:A:231:VAL:HG11	1:A:372:MET:HE1	1.92	0.51
1:A:85:LYS:HB3	3:A:5200:HOH:O	2.10	0.51
1:A:208:ASN:OD1	1:A:243:SER:HB2	2.11	0.51
1:A:516:PHE:O	1:A:520:LEU:HB2	2.11	0.51
1:A:456:SER:O	1:A:511:ILE:HG23	2.10	0.51
1:A:583:ALA:HB3	3:A:5341:HOH:O	2.09	0.51
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.93	0.50
1:B:104:LYS:HG3	1:B:187:GLN:NE2	2.26	0.50
1:B:84:GLN:HG3	1:B:88:GLU:OE1	2.11	0.50
1:B:161:GLU:N	1:B:170:MET:HE3	2.26	0.50
1:B:263:TYR:HE1	1:B:276:VAL:HG11	1.76	0.50
1:B:287:CYS:HB2	3:B:6202:HOH:O	2.11	0.50
1:A:624:ALA:HA	3:A:5351:HOH:O	2.11	0.50
1:A:361:TYR:HA	1:A:364:LYS:HE3	1.92	0.50
1:A:574:TYR:CZ	1:A:603:MET:HG3	2.46	0.50
1:B:136:LEU:HD21	1:B:237:TRP:CE3	2.46	0.50
1:A:321:ARG:CZ	1:A:330:ILE:HG21	2.41	0.50
1:A:487:VAL:HG13	1:A:491:GLN:OE1	2.10	0.50
1:A:45:GLN:NE2	1:A:514:GLU:HG2	2.25	0.50
1:B:88:GLU:HG2	3:B:6303:HOH:O	2.11	0.50
1:B:456:SER:HB2	2:B:6170:COA:H72	1.93	0.50

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:LYS:NZ	1:B:613:ASP:CG	2.64	0.50
1:B:104:LYS:CD	1:B:187:GLN:HE22	2.23	0.50
1:B:431:ALA:HB3	1:B:500:VAL:HG13	1.94	0.50
1:B:75:THR:HG23	1:B:78:GLY:HA3	1.93	0.50
1:A:144:GLU:HG2	1:A:361:TYR:CZ	2.47	0.50
1:A:104:LYS:HE3	1:A:187:GLN:NE2	2.26	0.49
1:A:263:TYR:HE1	1:A:276:VAL:HG11	1.77	0.49
1:B:70:VAL:O	1:B:74:GLN:HG2	2.12	0.49
1:A:95:GLU:OE1	1:A:462:LEU:HD11	2.12	0.49
1:A:263:TYR:O	1:A:267:ILE:HG12	2.13	0.49
1:A:366:GLU:HA	1:A:369:ARG:HH21	1.76	0.49
1:B:354:LEU:C	1:B:354:LEU:HD23	2.33	0.49
1:A:566:PHE:CE2	1:A:577:CYS:HB2	2.46	0.49
1:A:277:ASN:O	1:A:281:LYS:HG3	2.12	0.49
1:A:410:MET:SD	3:A:5309:HOH:O	2.60	0.49
1:B:209:TYR:CD1	1:B:247:PRO:HB3	2.46	0.49
1:A:93:LYS:O	1:A:94:MET:HG3	2.13	0.49
1:B:177:LEU:HD22	1:B:283:ILE:CG2	2.43	0.49
1:A:548:HIS:CE1	1:A:570:VAL:HG11	2.48	0.49
1:B:167:PRO:HD2	3:B:6285:HOH:O	2.12	0.49
1:A:230:PHE:O	1:A:234:GLU:HB2	2.13	0.49
1:A:553:THR:HG22	1:A:576:ILE:HB	1.95	0.49
1:A:295:VAL:HG12	1:A:296:SER:N	2.25	0.48
1:A:208:ASN:O	1:A:209:TYR:HB2	2.13	0.48
1:A:496:LEU:HG	1:A:614:MET:HE3	1.94	0.48
1:A:289:ASP:CG	1:A:321:ARG:HH12	2.16	0.48
1:A:355:VAL:HG12	3:A:5321:HOH:O	2.12	0.48
1:A:366:GLU:HB3	1:A:369:ARG:HE	1.78	0.48
1:A:123:ILE:O	1:A:562:CYS:HB2	2.14	0.48
1:A:86:GLY:HA2	1:A:89:ARG:NH2	2.28	0.48
1:A:296:SER:HB3	1:A:298:ASP:OD1	2.14	0.48
1:B:528:ILE:HG22	3:B:6247:HOH:O	2.12	0.48
1:B:66:THR:O	1:B:70:VAL:HG23	2.14	0.48
1:A:110:PHE:CZ	1:A:112:GLN:HB2	2.48	0.48
1:B:270:LYS:HG3	1:B:271:VAL:H	1.76	0.48
1:B:509:ARG:HG3	3:B:6251:HOH:O	2.14	0.48
1:A:225:THR:H	1:A:228:GLN:HE22	1.62	0.48
1:B:110:PHE:CE2	1:B:112:GLN:HB2	2.49	0.48
1:B:425:GLU:OE1	1:B:618:LEU:HD22	2.14	0.48
2:A:5170:COA:H8A	2:A:5170:COA:O2A	2.14	0.48
1:A:108:LEU:HD22	1:A:188:ASP:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ALA:N	3:B:6384:HOH:O	2.39	0.48
1:B:160:VAL:N	3:B:6263:HOH:O	2.47	0.48
1:B:90:ARG:HB2	3:B:6280:HOH:O	2.14	0.48
1:B:453:GLU:HA	1:B:553:THR:O	2.14	0.48
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.48	0.48
1:A:169:CYS:N	1:A:458:ARG:O	2.32	0.47
1:B:227:ASP:O	1:B:231:VAL:HG23	2.14	0.47
1:A:255:HIS:HD2	1:A:257:ASN:H	1.60	0.47
1:B:569:VAL:HG23	1:B:570:VAL:N	2.29	0.47
1:B:310:HIS:CD2	1:B:312:GLY:H	2.31	0.47
1:A:496:LEU:HD21	1:A:614:MET:CE	2.44	0.47
1:A:520:LEU:CD1	1:A:538:PHE:HE2	2.26	0.47
1:B:171:ASN:N	3:B:6288:HOH:O	2.47	0.47
1:B:407:LEU:HD21	1:B:409:ILE:HD11	1.96	0.47
1:B:321:ARG:HB3	1:B:328:GLN:HE22	1.78	0.47
1:A:414:PHE:CE2	1:A:611:LEU:HD13	2.49	0.47
1:A:289:ASP:OD1	1:A:317:ASN:HB3	2.15	0.47
1:A:269:ASP:HB3	1:A:272:ASN:HB2	1.97	0.47
1:A:584:HIS:O	1:A:585:ILE:HG13	2.14	0.47
1:A:294:ARG:NH1	1:A:294:ARG:HG3	2.28	0.47
1:A:65:HIS:CD2	3:A:5274:HOH:O	2.67	0.47
1:B:455:ALA:HB2	1:B:468:ILE:CG1	2.43	0.47
1:B:514:GLU:HG2	3:B:6282:HOH:O	2.14	0.47
1:A:366:GLU:CB	1:A:369:ARG:HH21	2.27	0.47
1:B:507:THR:O	1:B:511:ILE:HG13	2.14	0.47
1:B:115:VAL:O	1:B:116:ILE:HB	2.14	0.47
1:A:581:MET:HG3	1:A:584:HIS:CE1	2.50	0.47
1:A:198:ARG:HH12	1:A:281:LYS:HZ1	1.61	0.47
1:B:163:LEU:HD23	1:B:168:LEU:HD21	1.95	0.47
1:A:291:GLN:HG2	1:A:292:VAL:N	2.29	0.47
1:A:502:ALA:HA	3:A:5371:HOH:O	2.15	0.47
1:A:458:ARG:HD3	3:A:5267:HOH:O	2.15	0.47
1:B:300:TYR:O	1:B:304:VAL:HG23	2.15	0.47
1:A:587:PHE:CZ	1:A:607:LEU:HD21	2.49	0.47
1:B:129:PHE:HD2	3:B:6225:HOH:O	1.98	0.47
1:B:173:TYR:CZ	1:B:350:PRO:HA	2.50	0.46
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.96	0.46
1:A:437:LEU:HG	1:A:551:LEU:HD13	1.96	0.46
1:B:123:ILE:HD11	1:B:305:ALA:HB2	1.98	0.46
1:B:89:ARG:HD2	3:B:6356:HOH:O	2.14	0.46
1:A:207:HIS:O	1:A:208:ASN:HB2	2.15	0.46

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ILE:CG2	1:A:538:PHE:N	2.79	0.46
1:B:88:GLU:O	1:B:92:LYS:HG3	2.15	0.46
1:B:83:LEU:HD13	1:B:527:ALA:HB2	1.97	0.46
1:A:609:LYS:NZ	1:A:613:ASP:OD1	2.48	0.46
1:A:285:THR:HB	1:A:328:GLN:HG2	1.97	0.46
1:A:431:ALA:HA	1:A:503:HIS:ND1	2.30	0.46
1:A:442:TYR:OH	1:A:480:LYS:HG2	2.16	0.46
1:B:308:MET:CE	1:B:330:ILE:HG21	2.45	0.46
1:B:461:HIS:O	1:B:462:LEU:HB2	2.14	0.46
1:B:563:VAL:HB	1:B:586:ASN:HB3	1.97	0.46
1:A:90:ARG:HG2	1:A:94:MET:SD	2.55	0.46
1:A:160:VAL:HG13	3:A:5488:HOH:O	2.15	0.46
1:B:577:CYS:SG	1:B:578:TYR:N	2.89	0.46
1:B:118:SER:O	1:B:120:PRO:HD3	2.16	0.46
1:A:123:ILE:HD11	1:A:305:ALA:CA	2.46	0.46
1:A:197:LYS:C	1:A:199:PRO:HD3	2.36	0.46
1:B:285:THR:OG1	1:B:325:LYS:HG2	2.16	0.46
1:B:203:ILE:HA	1:B:282:SER:HB3	1.98	0.46
1:A:520:LEU:HA	1:A:520:LEU:HD22	1.67	0.46
1:B:210:GLN:HA	3:B:6300:HOH:O	2.14	0.46
1:A:466:ASP:HA	1:A:518:ARG:CZ	2.46	0.46
1:A:98:LEU:HD21	1:A:518:ARG:HB3	1.98	0.46
1:B:343:HIS:CE1	3:B:6252:HOH:O	2.68	0.46
1:B:207:HIS:HD2	1:B:240:SER:O	1.98	0.46
1:A:133:GLN:HE22	1:A:137:ARG:HG3	1.81	0.46
1:B:457:LEU:HA	3:B:6375:HOH:O	2.16	0.45
1:B:457:LEU:HG	1:B:466:ASP:HB2	1.98	0.45
1:A:163:LEU:HD22	1:A:168:LEU:HD21	1.98	0.45
1:B:31:HIS:CE1	1:B:167:PRO:HB3	2.51	0.45
1:A:90:ARG:O	1:A:94:MET:HB2	2.15	0.45
1:A:287:CYS:HB3	1:A:320:ASN:ND2	2.32	0.45
1:B:244:ASN:O	1:B:245:LYS:HD3	2.16	0.45
1:A:511:ILE:HG22	1:A:511:ILE:O	2.16	0.45
1:A:347:GLU:HB3	2:A:5170:COA:H32	1.98	0.45
1:A:283:ILE:O	1:A:284:PHE:HB3	2.16	0.45
1:B:85:LYS:O	1:B:89:ARG:HG3	2.17	0.45
1:B:420:ASP:HB3	1:B:582:GLU:O	2.16	0.45
1:B:489:GLU:HG2	1:B:617:LEU:HD11	1.98	0.45
1:B:225:THR:OG1	1:B:228:GLN:NE2	2.49	0.45
1:B:407:LEU:CD2	1:B:409:ILE:HD11	2.46	0.45
1:B:348:GLY:N	1:B:349:PRO:CD	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:MET:SD	1:A:378:PRO:HD2	2.55	0.45
1:A:238:ASN:HA	3:A:5349:HOH:O	2.16	0.45
1:B:586:ASN:C	3:B:6421:HOH:O	2.55	0.45
1:B:228:GLN:HE21	1:B:228:GLN:HB2	1.48	0.45
1:B:568:PRO:HD2	1:B:592:TYR:CE2	2.51	0.45
1:B:124:LEU:HG	1:B:338:GLY:HA2	1.98	0.45
1:A:425:GLU:O	1:A:427:LEU:HG	2.16	0.45
1:A:230:PHE:HB3	3:A:5205:HOH:O	2.16	0.45
1:B:41:PRO:HA	1:B:42:PRO:HD3	1.87	0.45
1:A:496:LEU:HD21	1:A:614:MET:HE2	1.99	0.45
1:A:224:LEU:HA	1:A:228:GLN:NE2	2.31	0.45
1:B:472:SER:HA	3:B:6350:HOH:O	2.16	0.45
1:B:44:GLN:HG2	1:B:74:GLN:OE1	2.17	0.45
1:A:475:SER:O	1:A:479:VAL:HG13	2.17	0.45
1:A:513:GLY:HA2	3:A:5254:HOH:O	2.16	0.45
1:B:452:TYR:CD2	1:B:452:TYR:C	2.90	0.45
1:A:35:LEU:HD21	1:A:167:PRO:HB2	1.99	0.45
1:A:118:SER:O	1:A:120:PRO:HD3	2.17	0.45
1:B:429:PRO:O	1:B:433:ILE:HG13	2.17	0.45
1:B:132:LEU:H	1:B:132:LEU:CD2	2.16	0.44
1:B:321:ARG:NE	1:B:330:ILE:HD11	2.32	0.44
1:A:415:HIS:CD2	1:A:416:HIS:N	2.85	0.44
1:A:225:THR:N	1:A:228:GLN:NE2	2.61	0.44
1:B:509:ARG:CB	1:B:514:GLU:HB2	2.47	0.44
1:A:168:LEU:HD22	1:A:458:ARG:CB	2.47	0.44
1:B:32:GLN:NE2	1:B:35:LEU:HD12	2.32	0.44
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.82	0.44
1:A:176:ILE:HA	1:A:326:THR:HG21	2.00	0.44
1:B:98:LEU:HD22	1:B:518:ARG:HB3	2.00	0.44
1:A:612:LEU:CD2	1:A:615:ARG:HH21	2.30	0.44
1:B:170:MET:HE1	1:B:458:ARG:NH2	2.33	0.44
1:B:229:ILE:HG22	1:B:233:LEU:HD11	1.99	0.44
1:A:555:GLN:OE1	1:A:557:PRO:HG3	2.17	0.44
1:B:155:ASN:O	1:B:156:GLU:HB2	2.17	0.44
1:B:369:ARG:O	1:B:370:SER:HB2	2.17	0.44
1:A:115:VAL:HA	3:A:5179:HOH:O	2.18	0.44
1:B:609:LYS:HZ2	1:B:613:ASP:CG	2.20	0.44
1:A:207:HIS:CD2	1:A:208:ASN:HD22	2.36	0.44
1:A:177:LEU:HB2	3:A:5183:HOH:O	2.18	0.44
1:B:385:ILE:HG22	1:B:386:THR:N	2.32	0.44
1:B:349:PRO:HB2	1:B:350:PRO:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:HA	1:B:506:TYR:CE2	2.53	0.44
1:A:112:GLN:HE21	1:A:113:PRO:HD3	1.83	0.44
1:B:84:GLN:HA	1:B:84:GLN:HE21	1.82	0.44
1:B:472:SER:HB3	3:B:6233:HOH:O	2.17	0.44
1:A:70:VAL:O	1:A:74:GLN:HG2	2.17	0.44
1:A:543:TYR:HB3	3:A:5454:HOH:O	2.17	0.44
1:B:333:GLU:CD	1:B:333:GLU:C	2.76	0.44
1:A:77:GLY:HA2	1:A:81:GLU:OE1	2.17	0.44
1:B:307:GLN:O	1:B:311:GLY:HA2	2.18	0.44
1:A:507:THR:O	1:A:511:ILE:HG13	2.18	0.44
1:A:37:ARG:HG3	1:A:95:GLU:O	2.18	0.44
1:B:31:HIS:HE1	1:B:167:PRO:HB3	1.83	0.44
1:B:72:GLU:HG3	1:B:72:GLU:O	2.17	0.44
1:A:419:LYS:HB3	1:A:423:LYS:HE2	2.00	0.44
1:B:90:ARG:HA	1:B:93:LYS:HE2	2.00	0.44
1:A:312:GLY:O	1:A:316:PHE:HD1	2.01	0.44
1:A:115:VAL:C	1:A:117:TYR:H	2.20	0.44
1:B:467:THR:CG2	1:B:468:ILE:N	2.80	0.44
1:B:400:LEU:HG	1:B:404:ILE:HD11	2.00	0.44
1:A:411:MET:CE	1:A:563:VAL:HG11	2.48	0.44
1:A:312:GLY:O	1:A:316:PHE:HB2	2.17	0.43
1:A:461:HIS:CE1	1:A:462:LEU:HG	2.53	0.43
1:B:308:MET:HE2	1:B:330:ILE:HG21	1.99	0.43
1:B:143:ILE:HB	1:B:229:ILE:HD13	2.00	0.43
1:A:404:ILE:C	1:A:406:ASP:H	2.20	0.43
1:A:505:ALA:O	1:A:509:ARG:HG3	2.18	0.43
1:A:405:GLN:HE21	1:A:405:GLN:HB2	1.67	0.43
1:A:458:ARG:HD3	3:A:5182:HOH:O	2.18	0.43
1:A:218:HIS:C	1:A:220:ASP:N	2.70	0.43
1:B:42:PRO:O	1:B:45:GLN:HB3	2.18	0.43
1:B:321:ARG:HE	1:B:330:ILE:HD11	1.83	0.43
1:B:119:SER:HB3	1:B:341:TYR:O	2.18	0.43
1:A:224:LEU:HA	1:A:228:GLN:HE22	1.83	0.43
1:A:104:LYS:HE2	1:A:109:GLN:OE1	2.18	0.43
1:B:294:ARG:HA	1:B:294:ARG:CZ	2.48	0.43
1:B:507:THR:CG2	2:B:6170:COA:H133	2.49	0.43
1:A:115:VAL:O	1:A:117:TYR:N	2.49	0.43
1:B:416:HIS:O	1:B:417:PHE:HB3	2.17	0.43
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.54	0.43
1:B:178:SER:H	1:B:283:ILE:HA	1.83	0.43
1:B:431:ALA:HB1	1:B:500:VAL:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:VAL:HG23	1:B:570:VAL:H	1.84	0.43
1:A:266:LEU:HD12	1:A:272:ASN:HD22	1.83	0.43
1:B:129:PHE:N	3:B:6225:HOH:O	2.51	0.43
1:A:497:ARG:NH1	1:A:623:ARG:HB2	2.34	0.43
1:B:308:MET:O	3:B:6171:HOH:O	2.21	0.43
1:B:467:THR:HG22	1:B:468:ILE:N	2.33	0.43
1:A:224:LEU:HB3	1:A:229:ILE:CG1	2.49	0.43
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.83	0.43
1:B:356:ASP:OD2	1:B:559:LYS:HB2	2.18	0.43
1:A:352:VAL:C	1:A:354:LEU:H	2.22	0.43
1:B:76:SER:C	1:B:78:GLY:N	2.73	0.43
1:A:429:PRO:O	1:A:433:ILE:HG13	2.18	0.43
1:A:90:ARG:O	1:A:90:ARG:HG2	2.19	0.42
1:B:108:LEU:HD13	1:B:188:ASP:O	2.18	0.42
1:A:456:SER:HA	1:A:465:THR:HG22	2.01	0.42
1:A:452:TYR:HB2	1:A:549:PHE:CD1	2.54	0.42
1:B:464:ARG:HA	1:B:464:ARG:HD2	1.84	0.42
1:B:410:MET:HB3	1:B:600:ALA:HB1	2.01	0.42
1:A:224:LEU:HG	1:A:228:GLN:CB	2.48	0.42
1:A:300:TYR:O	1:A:303:HIS:N	2.47	0.42
1:A:133:GLN:O	1:A:137:ARG:HG2	2.18	0.42
1:B:349:PRO:HA	3:B:6319:HOH:O	2.18	0.42
1:A:554:SER:CB	2:A:5170:COA:H22	2.48	0.42
1:B:49:TYR:CE2	1:B:509:ARG:NE	2.87	0.42
1:B:184:GLY:HA3	1:B:187:GLN:O	2.19	0.42
1:A:558:ALA:C	1:A:560:THR:H	2.23	0.42
1:B:496:LEU:HD22	1:B:618:LEU:HD11	2.00	0.42
1:B:131:ASP:OD2	1:B:133:GLN:HG2	2.19	0.42
1:B:462:LEU:O	3:B:6190:HOH:O	2.22	0.42
1:B:172:GLN:HB3	1:B:346:ALA:HB2	2.02	0.42
1:A:196:SER:O	1:A:199:PRO:HD3	2.20	0.42
1:A:64:ALA:O	1:A:67:LYS:HB3	2.20	0.42
1:A:548:HIS:HB3	3:A:5477:HOH:O	2.20	0.42
1:B:354:LEU:O	1:B:354:LEU:HD23	2.19	0.42
1:B:104:LYS:HE2	1:B:104:LYS:HB3	1.90	0.42
1:B:80:GLY:C	1:B:82:ARG:H	2.22	0.42
1:B:496:LEU:O	1:B:500:VAL:HG23	2.20	0.42
1:A:619:GLN:O	1:B:186:LYS:HD3	2.18	0.42
1:B:75:THR:OG1	1:B:76:SER:N	2.52	0.42
1:B:54:LEU:HD22	1:B:58:VAL:HG11	2.02	0.42
1:B:252:THR:OG1	1:B:323:PHE:HD1	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PHE:CE1	1:A:416:HIS:CD2	2.92	0.42
1:B:94:MET:HE3	1:B:97:TRP:HA	2.01	0.42
1:B:263:TYR:O	1:B:267:ILE:HG12	2.20	0.42
1:A:265:ASN:ND2	1:A:388:GLU:OE1	2.52	0.42
1:A:183:PRO:CG	1:A:259:TRP:CD1	3.03	0.42
1:A:489:GLU:HB3	1:A:621:HIS:NE2	2.35	0.42
1:B:90:ARG:NH2	3:B:6210:HOH:O	2.52	0.42
1:B:97:TRP:O	3:B:6178:HOH:O	2.22	0.42
1:A:224:LEU:HG	1:A:228:GLN:NE2	2.35	0.42
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.35	0.42
1:A:566:PHE:CZ	1:A:577:CYS:HB2	2.55	0.42
1:B:79:VAL:O	1:B:83:LEU:HG	2.20	0.42
1:B:55:GLN:HB3	1:B:56:PRO:HD3	2.02	0.42
1:A:407:LEU:HG	1:A:409:ILE:HD11	2.02	0.42
1:B:476:LEU:O	1:B:480:LYS:HG3	2.20	0.41
1:A:109:GLN:O	1:A:111:ARG:HG2	2.20	0.41
1:B:55:GLN:NE2	3:B:6330:HOH:O	2.52	0.41
1:A:457:LEU:HD12	1:A:460:PHE:CD1	2.54	0.41
1:A:430:ASP:HB2	1:A:555:GLN:HE22	1.84	0.41
1:A:452:TYR:CD1	1:A:467:THR:HG23	2.55	0.41
1:B:98:LEU:O	1:B:99:SER:C	2.59	0.41
1:B:565:PHE:HB3	1:B:588:SER:CB	2.51	0.41
1:A:126:LYS:NZ	1:A:334:ASP:O	2.53	0.41
1:B:445:TYR:OH	1:B:597:GLU:O	2.22	0.41
1:A:466:ASP:HA	1:A:518:ARG:NH1	2.35	0.41
1:A:417:PHE:O	1:A:584:HIS:HA	2.21	0.41
1:B:165:GLY:C	1:B:166:GLN:HG3	2.40	0.41
1:B:574:TYR:OH	1:B:598:THR:HA	2.20	0.41
1:A:301:ARG:HG3	1:A:411:MET:HG3	2.01	0.41
1:B:54:LEU:O	1:B:55:GLN:C	2.58	0.41
1:A:166:GLN:CD	1:A:166:GLN:N	2.74	0.41
1:A:94:MET:HB3	3:A:5362:HOH:O	2.21	0.41
1:A:230:PHE:O	1:A:234:GLU:N	2.54	0.41
1:A:183:PRO:HG3	1:A:259:TRP:CD1	2.55	0.41
1:B:456:SER:HB2	2:B:6170:COA:C7P	2.50	0.41
1:B:47:LEU:CD1	1:B:74:GLN:HB3	2.46	0.41
1:A:322:TRP:H	1:A:328:GLN:HE22	1.69	0.41
1:B:593:ASN:C	1:B:595:CYS:N	2.74	0.41
1:B:295:VAL:HG11	1:B:303:HIS:NE2	2.35	0.41
1:A:354:LEU:C	1:A:354:LEU:HD23	2.41	0.41
1:B:53:ALA:O	1:B:56:PRO:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:HB2	1:B:357:HIS:ND1	2.36	0.41
1:A:132:LEU:N	1:A:132:LEU:HD22	2.35	0.41
1:A:115:VAL:O	1:A:116:ILE:HB	2.21	0.41
1:B:94:MET:HG2	3:B:6207:HOH:O	2.19	0.41
1:A:518:ARG:HD3	1:A:518:ARG:HA	1.90	0.41
1:A:487:VAL:HA	1:A:488:PRO:HD3	1.91	0.41
1:A:497:ARG:NH2	3:A:5265:HOH:O	2.53	0.41
1:A:132:LEU:HD12	1:A:237:TRP:CH2	2.55	0.41
1:A:320:ASN:O	1:A:321:ARG:HD3	2.21	0.40
1:A:152:MET:CB	1:A:158:LEU:HD12	2.48	0.40
1:A:497:ARG:CZ	1:A:623:ARG:HB2	2.50	0.40
1:B:108:LEU:HD22	1:B:188:ASP:O	2.21	0.40
1:B:480:LYS:O	1:B:484:ASP:HB2	2.20	0.40
1:B:104:LYS:HD3	3:B:6362:HOH:O	2.21	0.40
1:A:214:LEU:HD22	1:A:236:ILE:HD12	2.04	0.40
1:B:252:THR:HG22	1:B:259:TRP:CZ2	2.57	0.40
1:B:491:GLN:O	1:B:494:GLU:HB2	2.21	0.40
1:B:229:ILE:HG22	1:B:233:LEU:CD1	2.51	0.40
1:A:236:ILE:HG13	1:A:378:PRO:HG2	2.04	0.40
1:A:59:SER:HB3	1:A:62:GLU:CG	2.51	0.40
1:A:427:LEU:HB3	1:A:500:VAL:HG11	2.04	0.40
1:A:119:SER:HA	1:A:120:PRO:HD3	1.85	0.40
1:A:129:PHE:CE1	1:A:335:GLY:HA2	2.56	0.40
1:B:176:ILE:HG13	1:B:177:LEU:HG	2.03	0.40
1:A:322:TRP:N	1:A:328:GLN:HE22	2.20	0.40
1:B:31:HIS:CE1	1:B:160:VAL:HG11	2.56	0.40
1:B:451:THR:HG23	1:B:551:LEU:CB	2.45	0.40
1:B:512:ARG:CG	1:B:512:ARG:HH11	2.35	0.40
1:A:404:ILE:C	1:A:406:ASP:N	2.74	0.40
1:A:480:LYS:O	1:A:484:ASP:HB2	2.21	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	594/596 (100%)	501 (84%)	81 (14%)	12 (2%)	9	7
1	B	594/596 (100%)	532 (90%)	52 (9%)	10 (2%)	11	10
All	All	1188/1192 (100%)	1033 (87%)	133 (11%)	22 (2%)	10	8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	SER
1	B	515	ALA
1	B	485	SER
1	B	622	PRO
1	A	172	GLN
1	A	219	SER
1	A	244	ASN
1	A	284	PHE
1	A	371	PRO
1	B	196	SER
1	B	345	ALA
1	B	368	VAL
1	B	600	ALA
1	A	116	ILE
1	A	296	SER
1	B	367	LEU
1	A	76	SER
1	B	139	ALA
1	A	340	VAL
1	A	349	PRO
1	A	567	GLY
1	A	365	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	A	524/524 (100%)	494 (94%)	30 (6%)	25	34
1	B	524/524 (100%)	502 (96%)	22 (4%)	36	49
All	All	1048/1048 (100%)	996 (95%)	52 (5%)	30	41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	89	ARG
1	A	98	LEU
1	A	112	GLN
1	A	133	GLN
1	A	141	LYS
1	A	166	GLN
1	A	191	VAL
1	A	192	ASN
1	A	204	THR
1	A	220	ASP
1	A	224	LEU
1	A	227	ASP
1	A	275	SER
1	A	277	ASN
1	A	303	HIS
1	A	330	ILE
1	A	342	GLU
1	A	390	LYS
1	A	409	ILE
1	A	415	HIS
1	A	424	SER
1	A	454	SER
1	A	459	MET
1	A	482	MET
1	A	504	ARG
1	A	517	ASP
1	A	520	LEU
1	A	603	MET
1	A	625	LYS
1	B	132	LEU
1	B	144	GLU
1	B	163	LEU
1	B	192	ASN
1	B	202	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	THR
1	B	206	VAL
1	B	228	GLN
1	B	242	GLN
1	B	264	ASN
1	B	270	LYS
1	B	307	GLN
1	B	315	LYS
1	B	333	GLU
1	B	340	VAL
1	B	347	GLU
1	B	360	GLU
1	B	456	SER
1	B	470	SER
1	B	536	ASP
1	B	581	MET
1	B	619	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	45	GLN
1	A	55	GLN
1	A	65	HIS
1	A	84	GLN
1	A	112	GLN
1	A	133	GLN
1	A	135	GLN
1	A	192	ASN
1	A	208	ASN
1	A	228	GLN
1	A	255	HIS
1	A	265	ASN
1	A	277	ASN
1	A	307	GLN
1	A	310	HIS
1	A	320	ASN
1	A	328	GLN
1	A	399	ASN
1	A	405	GLN
1	A	415	HIS

Continued from previous page...

Mol	Chain	Res	Type
1	A	416	HIS
1	A	461	HIS
1	A	501	GLN
1	A	550	ASN
1	A	586	ASN
1	A	619	GLN
1	B	31	HIS
1	B	84	GLN
1	B	109	GLN
1	B	112	GLN
1	B	133	GLN
1	B	135	GLN
1	B	171	ASN
1	B	187	GLN
1	B	192	ASN
1	B	207	HIS
1	B	210	GLN
1	B	228	GLN
1	B	244	ASN
1	B	255	HIS
1	B	280	GLN
1	B	310	HIS
1	B	328	GLN
1	B	416	HIS
1	B	490	GLN
1	B	501	GLN
1	B	526	GLN
1	B	586	ASN
1	B	619	GLN
1	B	620	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	#$|Z| > 2$
2	COA	A	5170	-	40,50,50	1.25	2 (5%)	50,75,75	1.91	5 (10%)
2	COA	B	6170	-	40,50,50	1.15	2 (5%)	50,75,75	1.87	4 (8%)

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
2	COA	A	5170	-	-	0/44/64/64	0/3/3/3
2	COA	B	6170	-	-	0/44/64/64	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5170	COA	P3B-O7A	3.32	1.62	1.51
2	B	6170	COA	P3B-O7A	3.41	1.62	1.51
2	B	6170	COA	O4B-C1B	4.06	1.46	1.41
2	A	5170	COA	O4B-C1B	4.54	1.46	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6170	COA	N3A-C2A-N1A	-10.90	120.55	128.89
2	A	5170	COA	N3A-C2A-N1A	-10.88	120.56	128.89
2	A	5170	COA	P2A-O3A-P1A	-3.73	122.25	132.73

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6170	COA	P2A-O3A-P1A	-3.48	122.94	132.73
2	A	5170	COA	C5B-C4B-C3B	-2.23	106.28	114.31
2	B	6170	COA	O4B-C1B-N9A	2.96	114.30	108.10
2	B	6170	COA	O9A-P3B-O8A	3.10	119.17	107.38
2	A	5170	COA	O9A-P3B-O8A	3.15	119.39	107.38
2	A	5170	COA	O4B-C1B-N9A	3.41	115.25	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5170	COA	5	0
2	B	6170	COA	7	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(Å²)	Q<0.9
1	A	596/596 (100%)	0.29	26 (4%)	38	47	13, 47, 89, 134	0
1	B	596/596 (100%)	0.13	14 (2%)	64	72	14, 42, 72, 99	0
All	All	1192/1192 (100%)	0.21	40 (3%)	49	58	13, 44, 85, 134	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	ALA	9.0
1	A	373	VAL	7.3
1	A	367	LEU	6.9
1	A	371	PRO	5.7
1	A	370	SER	5.1
1	A	368	VAL	5.0
1	A	369	ARG	4.8
1	A	383	PHE	4.1
1	B	162	PHE	3.9
1	A	372	MET	3.7
1	A	374	PRO	3.6
1	A	162	PHE	3.4
1	B	165	GLY	3.3
1	B	365	PRO	3.3
1	B	367	LEU	3.3
1	B	30	ALA	3.2
1	B	625	LYS	3.0
1	B	160	VAL	2.9
1	B	68	GLN	2.9
1	A	364	LYS	2.9
1	A	241	LEU	2.8
1	A	366	GLU	2.8
1	A	625	LYS	2.7
1	B	63	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	198	ARG	2.5
1	A	624	ALA	2.5
1	A	250	ILE	2.5
1	B	31	HIS	2.5
1	A	294	ARG	2.4
1	A	376	PRO	2.4
1	A	146	VAL	2.3
1	A	365	PRO	2.2
1	A	230	PHE	2.1
1	A	133	GLN	2.1
1	B	378	PRO	2.1
1	A	237	TRP	2.1
1	A	242	GLN	2.0
1	B	504	ARG	2.0
1	B	166	GLN	2.0
1	A	386	THR	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	COA	A	5170	48/48	0.91	0.13	0.13	39,54,60,62	0
2	COA	B	6170	48/48	0.92	0.13	-0.39	36,53,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.